FINAL

BENCHMARKING/VERIFICATION OF TETRAD SIMULATOR, VERSION 12.7MS

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1 INTRODUCTION

The TETRAD simulator is a three-dimensional, multi-purpose simulation code that was first developed for petroleum reservoir and geothermal applications (Shook and Faulder, 1991; Vinsome and Shook, 1993), but was later modified for environmental applications by adding features such as dispersion/diffusion, adsorption, and decay (Shook, 1995). This modified version of the TETRAD code was used to evaluate the fate and transport of contaminants during the Operable Unit 7-13/14 (OU 7-13/14) remedial investigation (Magnuson and Sondrup, 2006). The application of TETRAD to OU 7-13/14 involves complex three-dimensional simulations in the vadose zone and in groundwater. The results of these simulations are used as a basis for conclusions and recommendations regarding how to best remediate subsurface conditions at OU 7-13/14. Because OU 7-13/14 is a significant and long term environmental concern, assurances of the reliability of the TETRAD computer code need to be fully documented.

Although TETRAD is a well known code, the testing and validation documentation is not complete or available for the most recent version. TETRAD has been extensively benchmarked for geothermal applications (Shook and Faulder, 1991; Vinsome and Shook, 1993), but much less so for environmental applications (Shook, 1995, Becker et al., 1996). The environmental problems are limited to two dimensions and consist of one comparison with variation of parameters to an analytical solution for solute transport (Shook, 1995) and two comparisons for hypothetical problems in the vadose zone (Shook, 1995, Becker et al., 1996). The TETRAD simulator has undergone numerous revisions over two decades. Based on the version history described in the TETRAD User Manual, testing of environmental applications of the code were most likely performed using version 10. However, for the OU 7-13/14 application, version 12.7ms was used. A comparison of results between version 12.7 and 12.7ms accounted for many conditions applicable to the OU 7-13/14 assessment, but otherwise it is not documented whether any attempt was made to rerun benchmark problems as versions have evolved.

Therefore, GeoTrans, Inc. (GeoTrans) selected a series of verification and benchmark problems to assess the reliability and functionality of the TETRAD Version 12.7ms computer code for simulating environmental fate and transport processes similar to those in the OU 7-13/14 application. Verification and benchmarking were accomplished by assessing the results of the TETRAD simulator on a series of benchmark problems that have been previously developed for environmental fate and transport codes. These benchmark problems test advection, dispersion, retardation, chain decay, and density driven flow in groundwater, flow and transport in the vadose zone, and flow and transport in dual porosity media in one-, two-, and three-dimensions.

In a letter dated May 12, 2006 GeoTrans, Inc. provided the Idaho National Laboratory (INL) with ten benchmark problems involving flow and transport in saturated, unsaturated, and fractured media that are appropriate to test the TETRAD computer code. These benchmark problems test for advection, dispersion, diffusion, retardation, chain decay, and density driven flow in groundwater; flow and transport in the vadose zone; and flow and transport in dual porosity media. An eleventh problem involving three-dimensional flow and transport of carbon tetrachloride was subsequently sent to INL in a letter dated July 20, 2006. A summary of the eleven selected benchmark problems are provided in Table 1.1.

Table 1.1. Summary of Benchmark Problems Selected by GeoTrans.

Problem #	Problem Description	Dimension	Problem Source
Problems that were simulated			
1	Transport with Chain Decay in Porous Media	1-D	Ross et al., 1982
2	Transport Between Injection and Production Wells with Chain Decay in Porous Media	2-D	Ross et al., 1982
3	Transport with Chain Decay in Fractured Porous Media	1-D	Ross et al., 1982
4	Hydrodynamic Dispersion During Absorption of Water by Soil	1-D	Ross et al., 1982
5	Flow and Solute Transport in the Unsaturated Zone	2-D	Ross et al., 1982
6	Transport of Injectate in a Variably Dipping Aquifer	2-D	DuPont, 1999a
7	Transport of Injectate in a Dipping Aquifer with a Background Velocity	2-D	DuPont, 1999b
8	Multiphase Carbon Tetrachloride Transport in Unsaturated and Saturated Media	3-D	Ross et al., 1982
Problems that were selected, but not simulated			
9	Flow and Transport of Waste in a Hypothetical Basalt Repository	3-D	Ross et al., 1982
10	Transport Between Injection and Production Wells with Chain Decay in Fractured Porous Media	2-D	Ross et al., 1982
11	Field Study: Tilmanstone, Kent, UK	3-D	Ross et al., 1982

TETRAD simulation results for eight of the benchmark problems were provided by INL to GeoTrans to review. Three of the problems were not simulated due to several considerations, including complexity, redundancy with other problems, and/or inadequacy of details necessary for problem set-up. The eight problems that were finally simulated address all of the processes and dimensionality appropriate for the OU 7-13/14 application.

2 PROBLEM 1 - TRANSPORT WITH CHAIN DECAY IN POROUS MEDIA

2.1 PROBLEM STATEMENT AND OBJECTIVES

A summary of this problem including project description, assumptions, input specifications, governing equations, and details on an analytical solution are presented in Ross et al. (1982). This problem corresponds to Problem 1 of INTRACOIN (1984) and Problem 8.1 of Ross et al. (1982). INTRACOIN was a study by the Swedish Nuclear Power Inspectorate (Statens Karnkraftinspektion) focusing in part on the numerical accuracy of radionuclide transport codes. The analytical solution for this problem was given by Harada et al. (1980).

As described in Ross et al. (1982), the main objective of this problem is to test the capability of a computer code to simulate one-dimensional convection, hydrodynamic dispersion, adsorption, radioactive decay, and chain reactions of a three member chain of radionuclides in a confined aquifer. A second objective is to test a number of conditions which can cause numerical difficulties, such as very large or small Peclet numbers, daughter products that move faster or slower and have much longer or shorter half-lives than parents, and daughter nuclides with half-lives on the same scale as their transit times.

In this problem, the three radionuclides are input at one end of the model domain at a constant rate (except for the effects of radioactive decay) over a specified period of time. Assumptions include 1) one-dimensional flow and transport, 2) the domain is semi-infinite, 3) groundwater velocity, retardation factors, and dispersivity are constant and uniform in each individual simulation, 4) solute transport occurs through advection and mechanical dispersion, 4) instantaneous changes in concentration penetrate the entire aquifer thickness, and 5) sorption is at equilibrium.

In addition to an analytical solution, this problem has been simulated using the Sandia Waste-Isolation Flow and Transport (SWIFT), NUTRAN, and NWFT/DVM computer codes.

SWIFT is a finite-difference, fully-coupled, transient, three-dimensional flow and transport model. The SWIFT model was initially developed for the U.S. Geological Survey beginning in 1975 (INTERCOMP, 1976) and incorporated fluid flow, heat transport, and fluid compositional changes for a miscible component (brine migration). The code was updated by Sandia Laboratories beginning in 1977 with the addition of radionuclide chain decay and transport (Dillon et al., 1978). Further improvements and additions have been made to the code over time, such as the SWIFT II code, which incorporates flow and transport properties in both fractured and porous media (Reeves et al., 1986).

NUTRAN, which was developed by The Analytic Sciences Corporation, Inc., is a flow path network code for simulating groundwater flow and radionuclide transport and evaluating associated dose to man consequences (Ross & Koplik, 1979; Ross et al., 1983). Fluid flow is analyzed using the electrical resistivity network law analogy to evaluate flow along a network of one-dimensional paths.

The Network Flow and Transport/Distributed Velocity (NWFT/DVM) code, which was developed by Sandia National Laboratories, is a flow path network code designed to simulate groundwater flow and radionuclide transport in a nuclear waste repository and surrounding geologic media (Cambell et al., 1981; Duda, 1984). The code uses a network presentation based on an electrical analog to simulate fluid flow in and around a repository.

2.2 INPUT SPECIFICATIONS

Twelve cases involving two radionuclide inventories, three dispersivities, and two sets of retardation factors have previously been simulated using the SWIFT, NUTRAN, and/or NWFT/DVM computer codes. The twelve cases are summarized in Table 2.1.

Table 2.1. Summary of Problem 1 Simulations.

Case #	Case Summary
Case 1	Inventory 1, Retardation Factor Set 1, Dispersivity 1
Case 2	Inventory 1, Retardation Factor Set 1, Dispersivity 2
Case 3	Inventory 1, Retardation Factor Set 1, Dispersivity 3
Case 4	Inventory 1, Retardation Factor Set 2, Dispersivity 1
Case 5	Inventory 1, Retardation Factor Set 2, Dispersivity 2
Case 6	Inventory 1, Retardation Factor Set 2, Dispersivity 3
Case 7	Inventory 2, Retardation Factor Set 1, Dispersivity 1
Case 8	Inventory 2, Retardation Factor Set 1, Dispersivity 2
Case 9	Inventory 2, Retardation Factor Set 1, Dispersivity 3
Case 10	Inventory 2, Retardation Factor Set 2, Dispersivity 1
Case 11	Inventory 2, Retardation Factor Set 2, Dispersivity 2
Case 12	Inventory 2, Retardation Factor Set 2, Dispersivity 3

Input parameters including the inventory, retardation factor, and dispersivity sets, which are provided in Ross et al. (1982), are summarized in Table 2.2.

Table 2.2. Input Parameters for Problem 1.

Parameter	**Nuclide**	**Half-life (yr)**	**Initial Inventory (Ci)**	**Initial Inventory (kg)**	**Retardation Factor Set 1**	**Retardation Factor Set 2**
Inventory 1	^{234}U	2.445×10^5	1.0	0.158	300	60
	^{230}Th	7.7×10^4	0.01	4.9×10^{-4}	2×10^4	500
	^{226}Ra	1.6×10^3	0.004	4.0×10^{-6}	1×10^4	20
Inventory 2	^{245}Cm	8.5×10^3	0.7	4.0×10^{-3}	5000	60
	^{237}Np	2.14×10^6	1.0	1.4	700	200
	^{233}U	1.592×10^5	0.004	4.1×10^{-4}	300	60

Parameter	**Value**	**Units**
Groundwater velocity	1	m/yr
Effective porosity	0.01	
Cross-sectional area of flow	100	m^2
Leach duration	10^5	yr
Dispersivity 1	0	m
Dispersivity 2	50	m
Dispersivity 3	500	m

Information on the SWIFT model discretization and other input parameters are provided in Ward et al. (1984). Information on the NUTRAN and NWFT/DVM model discretization and other input parameters are provided in the Benchmarking of Flow and Transport Codes For Licensing Assistance report by GeoTrans (1988).

2.3 COMPARISON OF RESULTS

SWIFT results of four of the twelve simulation cases (Cases 2, 5, 8, and 11) involving inventory sets 1 and 2, retardation factor sets 1 and 2, and dispersivity set 2 (50 meters) are published in Ward et al. (1984). The SWIFT results were comparable to the results of the analytical code UCB-NE (Harada et al., 1980). NUTRAN results for four of the twelve cases (Cases 3, 6, 9, and 12) involving inventory sets 1 and 2, retardation factor sets 1 and 2, and dispersivity set 3 (500 meters) are published in GeoTrans (1988). The NUTRAN results were compared to results from the analytical code UCB-NE, which were summarized in the INTRACOIN (1983) study. In general, agreement between NUTRAN and the analytic code were excellent for long-lived radionuclides with lesser agreement for fast decaying radionuclides or radionuclides with half-lives comparable to transport rates (GeoTrans, 1988). NWFT/DVM results for all twelve cases were published in GeoTrans (1988). The NWFT/DVM results were compared to the analytical code UCB-NE and the finite-difference code SWENT, which were summarized in the INTRACOIN (1983) study. In general, agreement between NWFT/DVM and UCB-NE and SWENT was good, although there was better agreement with the analytical code at a smaller Peclet number and better agreement with the finite-difference code at a larger Peclet number (GeoTrans, 1988).

INL provided simulation results consisting of concentration over time for all three radionuclides. A copy of the INL simulation results for all twelve cases is provided in Attachment 1. The results of all cases were plotted against concentrations calculated by the SWIFT, NUTRAN, and/or NWFT/DVM codes. Plots showing a comparison of these results are presented in Figures 2.1 to 2.12.

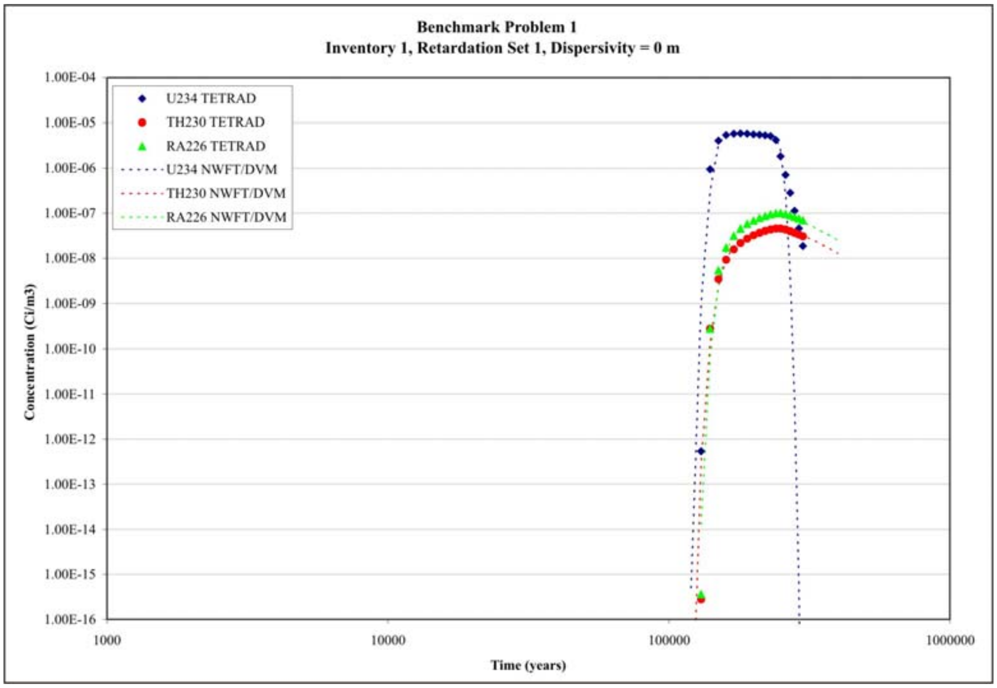

Figure 2.1. Comparison between TETRAD and NWFT/DVM simulation results for Problem 1, Case 1.

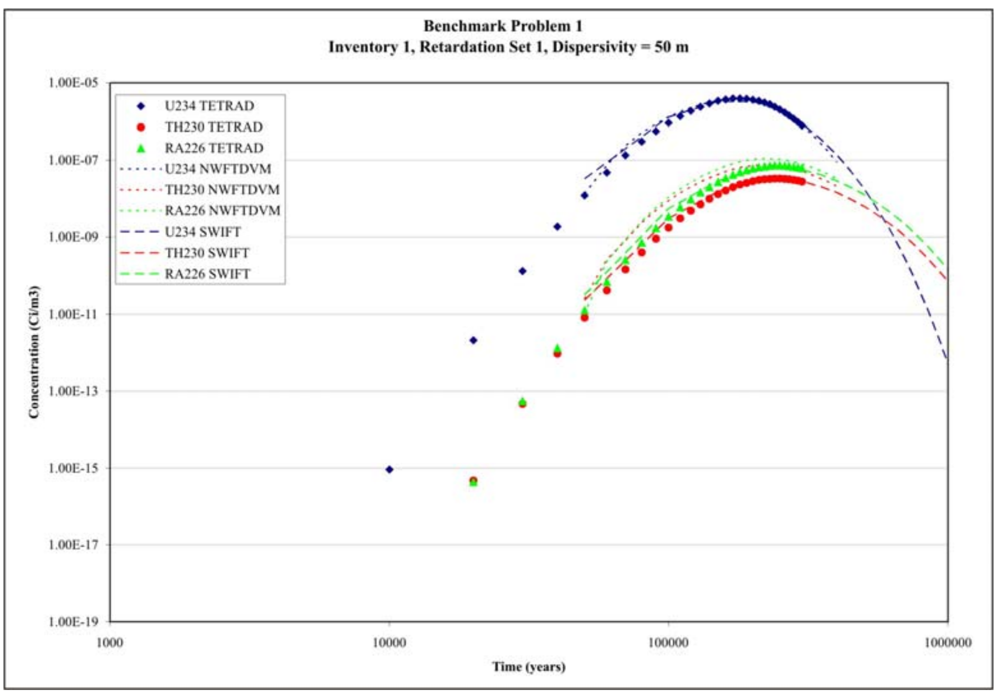

Figure 2.2. Comparison between TETRAD, SWIFT, and NWFT/DVM simulation results for Problem 1, Case 2.

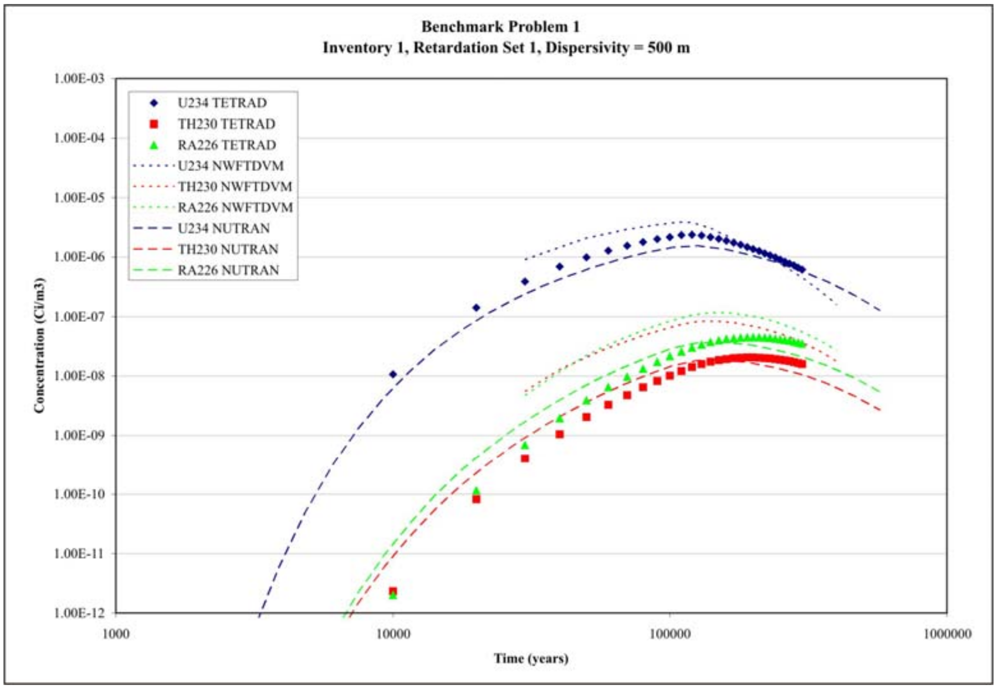

Figure 2.3. Comparison between TETRAD, NUTRAN, and NWFT/DVM simulation results for Problem 1, Case 3.

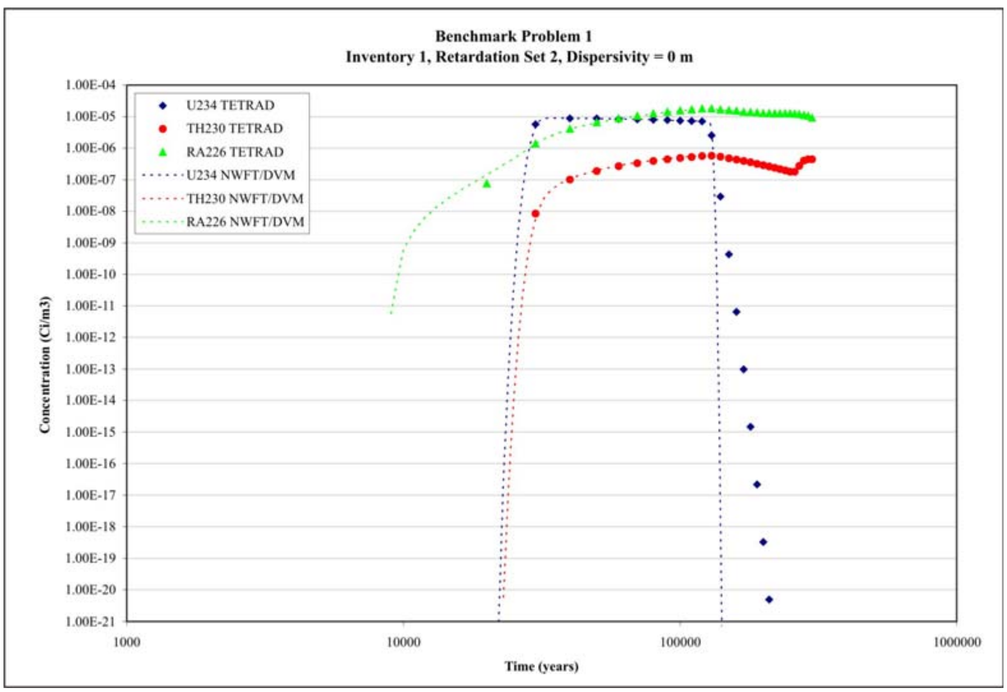

Figure 2.4. Comparison between TETRAD and NWFT/DVM simulation results for Problem 1, Case 4.

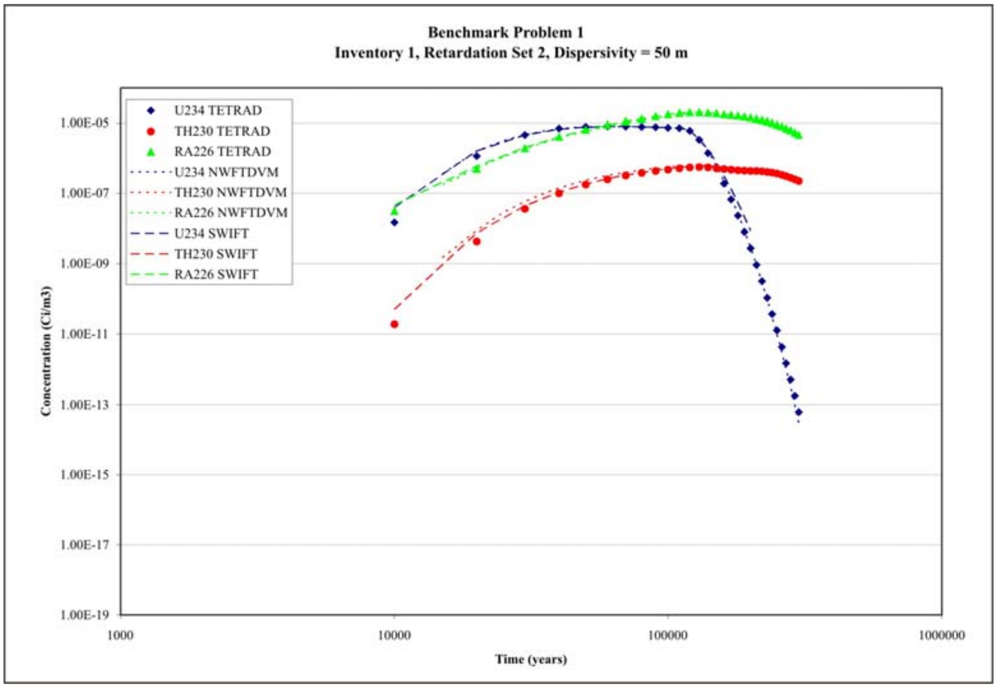

Figure 2.5. Comparison between TETRAD, SWIFT, and NWFT/DVM simulation results for Problem 1, Case 5.

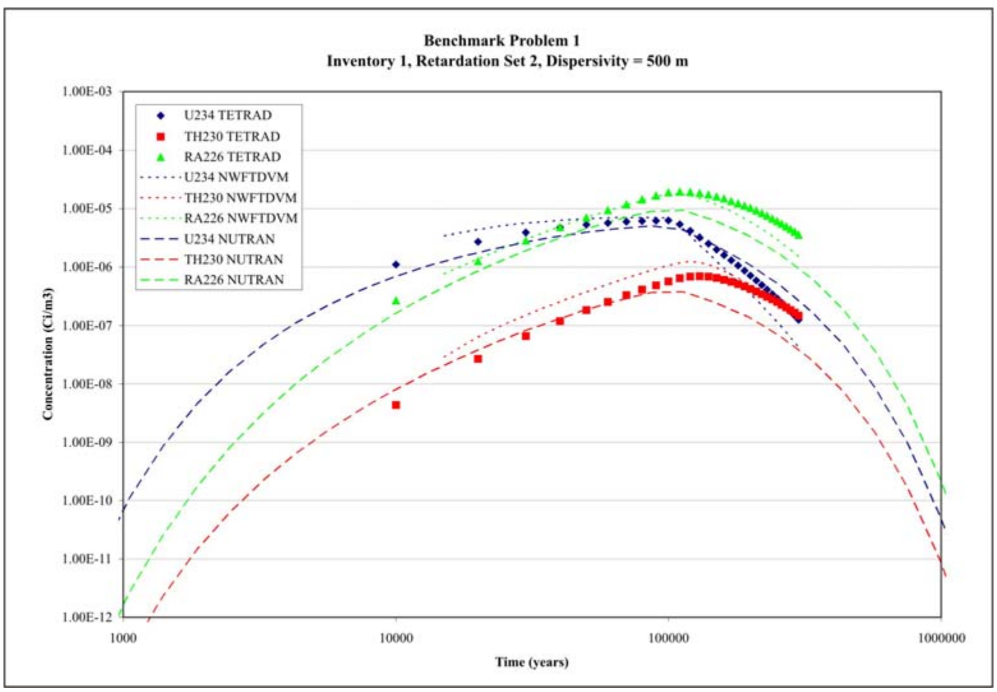

Figure 2.6. Comparison between TETRAD, NUTRAN, and NWFT/DVM simulation results for Problem 1, Case 6.

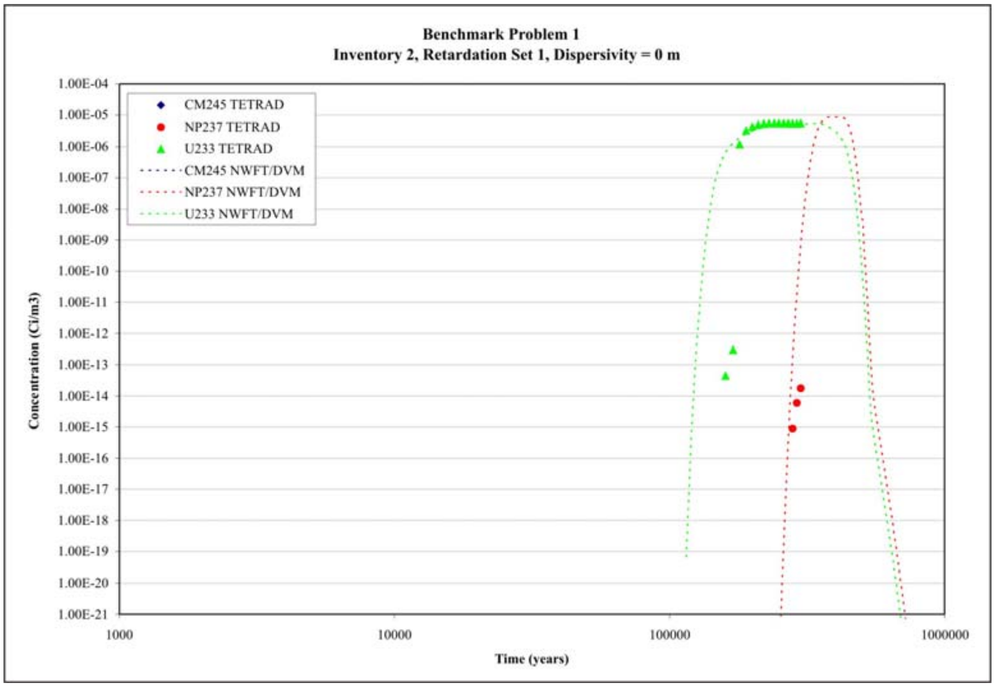

Figure 2.7. Comparison between TETRAD and NWFT/DVM simulation results for Problem 1, Case 7.

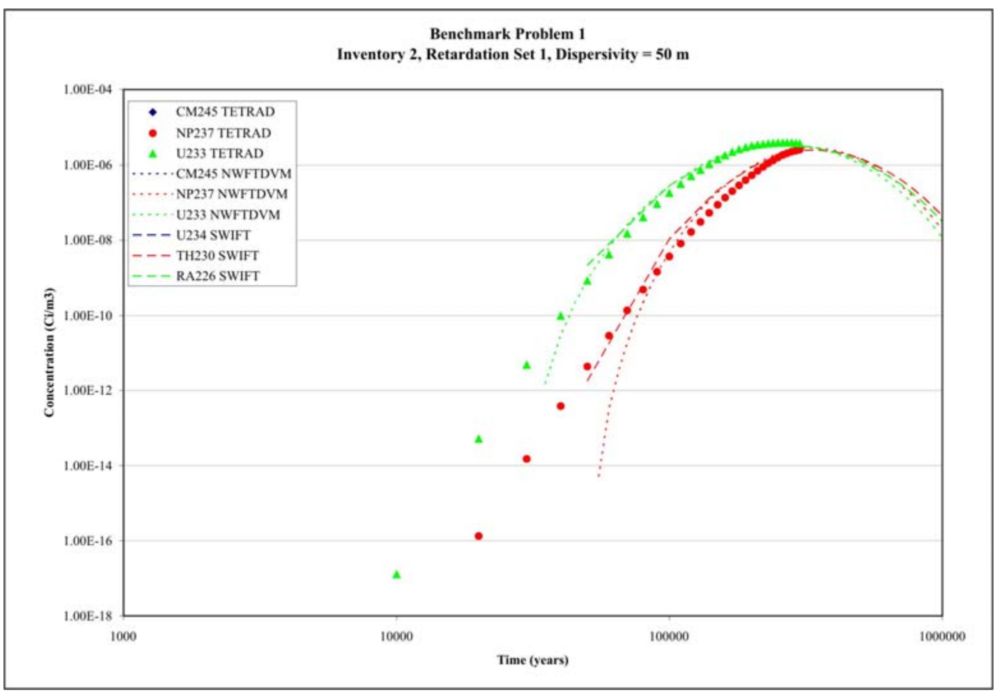

Figure 2.8. Comparison between TETRAD, SWIFT, and NWFT/DVM simulation results for Problem 1, Case 8.

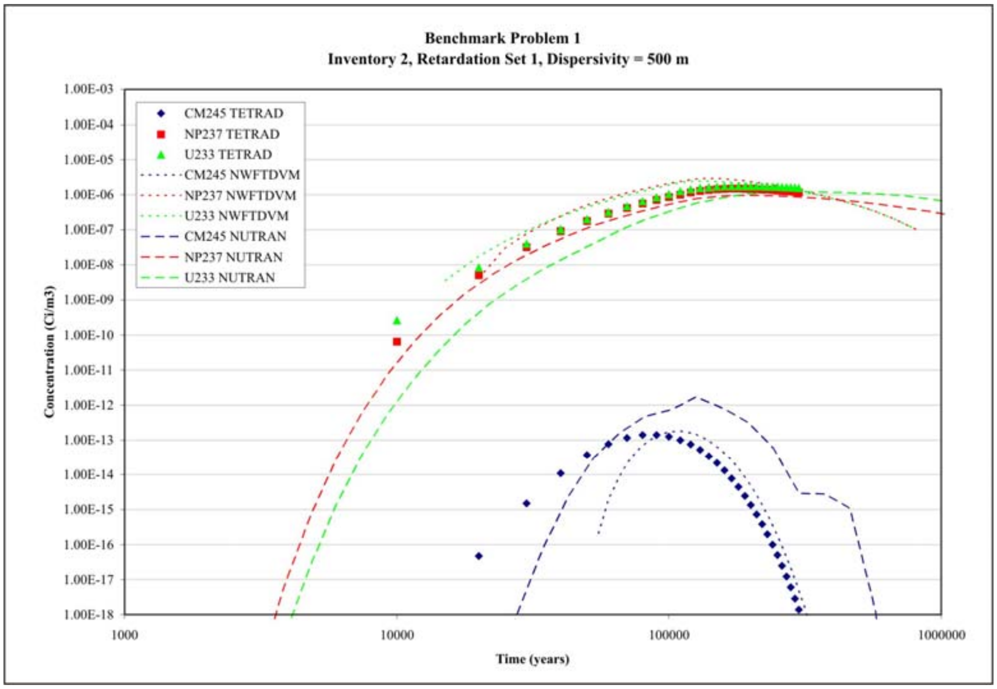

Figure 2.9. Comparison between TETRAD, NUTRAN, and NWFT/DVM simulation results for Problem 1, Case 9.

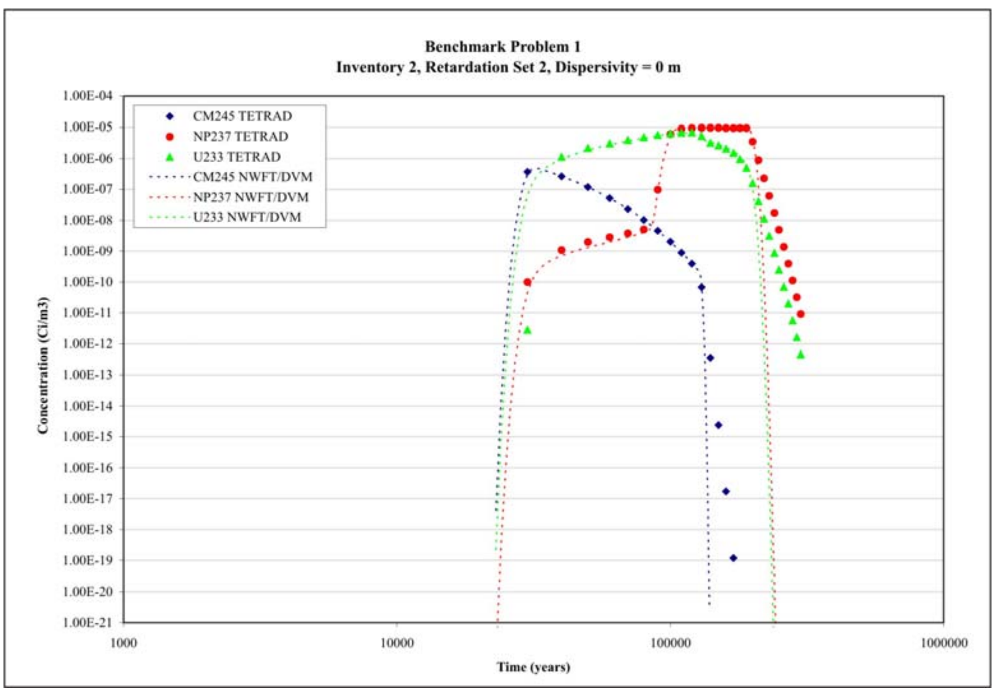

Figure 2.10. Comparison between TETRAD and NWFT/DVM simulation results for Problem 1, Case 10.

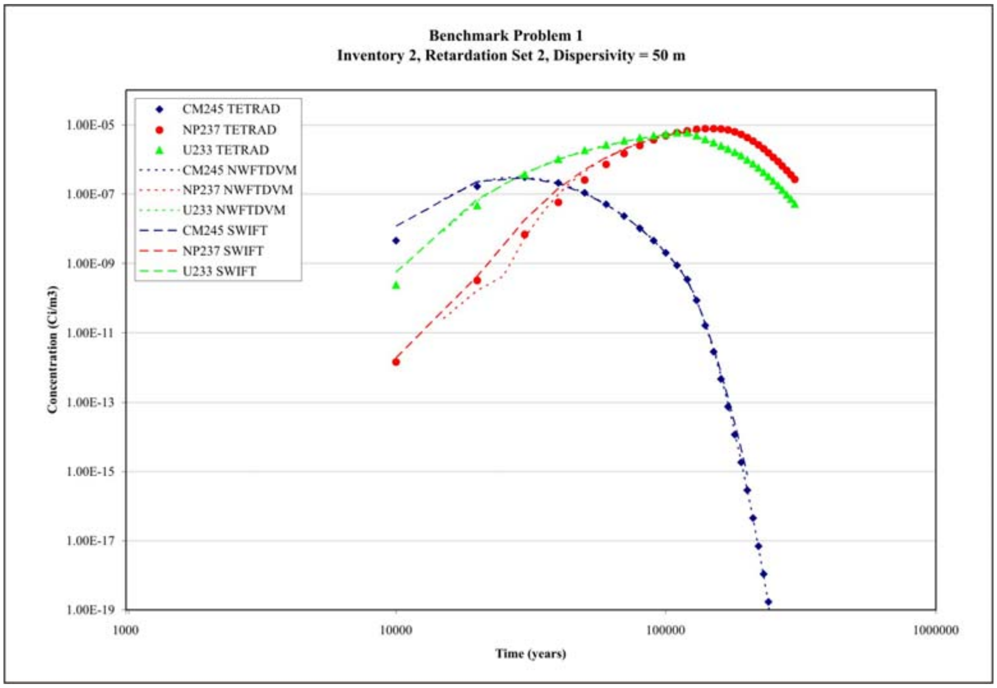

Figure 2.11. Comparison between TETRAD, SWIFT, and NWFT/DVM simulation results for Problem 1, Case 11.

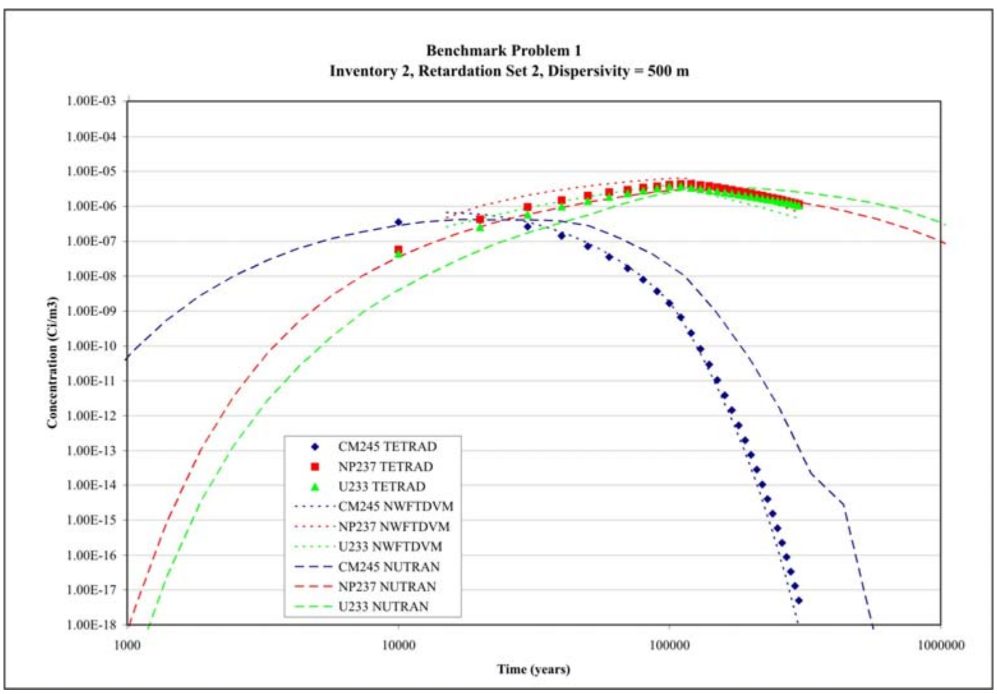

Figure 2.12. Comparison between TETRAD, NUTRAN, and NWFT/DVM simulation results for Problem 1, Case 12.

3 PROBLEM 2 - TRANSPORT BETWEEN INJECTION AND PRODUCTION WELLS WITH CHAIN DECAY IN POROUS MEDIA

3.1 PROBLEM STATEMENT AND OBJECTIVES

A summary of this problem including project description, assumptions, input specifications, and governing equations are presented in Ross et al. (1982). This problem corresponds to Problem 4b of INTRACOIN (1984) and Problem 8.2 of Ross et al. (1982).

This problem consists of two-dimensional flow and transport of a three-member radionuclide decay chain in a semi-infinite aquifer that contains an injection and extraction well and a contaminant source located between the two wells. The main objectives of the problem are 1) to test the capability of the computer code to simulate transport with chain decay in a non-uniform flow field and 2) to assess the reliability and accuracy of the time stepping scheme employed in the code. Assumptions include 1) the aquifer is uniform and isotropic, 2) no natural gradients are present, 3) the injection and extraction wells and the contaminant source fully penetrate the aquifer, and 4) the wells have been pumped for a sufficient time to establish steady-state groundwater flow before contaminant release begins.

The problem has been simulated using the SWIFT numerical code. A description of the SWIFT code is presented in Section 2.1.

3.2 INPUT SPECIFICATIONS

This problem uses radionuclide inventory set 1 and retardation factor set 2 presented in Table 2.2. Other input parameters, which are provided in Ross et al. (1982), are presented in Table 3.1.

Table 3.1. Input parameters for Problem 2.

Parameter	Value	Units
Release Duration	10^5	yr
Aquifer Thickness	100	m
Effective porosity	0.01	
Distance from origin to well	510	m
Pumping rate	1088.9	m^3/yr
Longitudinal dispersivity	50	m
Transverse dispersivity	5	m

Information on the SWIFT model discretization and other input parameters are provided in Ward et al. (1984).

3.3 Comparison of Results

Results of the SWIFT simulation for this problem are published in Ward et al. (1984). Results were provided for three points on the breakthrough curves: the peak flux rate and the two half-maximum rates that occur before and after the peak, and for the nuclide flux rate over time through the y-axis.

INL provided TETRAD simulation results consisting of concentration over time and distance along the Y-axis for all three radionuclides. A copy of the INL simulation results for Problem 2 is provided in Attachment 1. These results were plotted against concentrations calculated by the SWIFT code. A comparison of these results are presented in Figures 3.1 and 3.2.

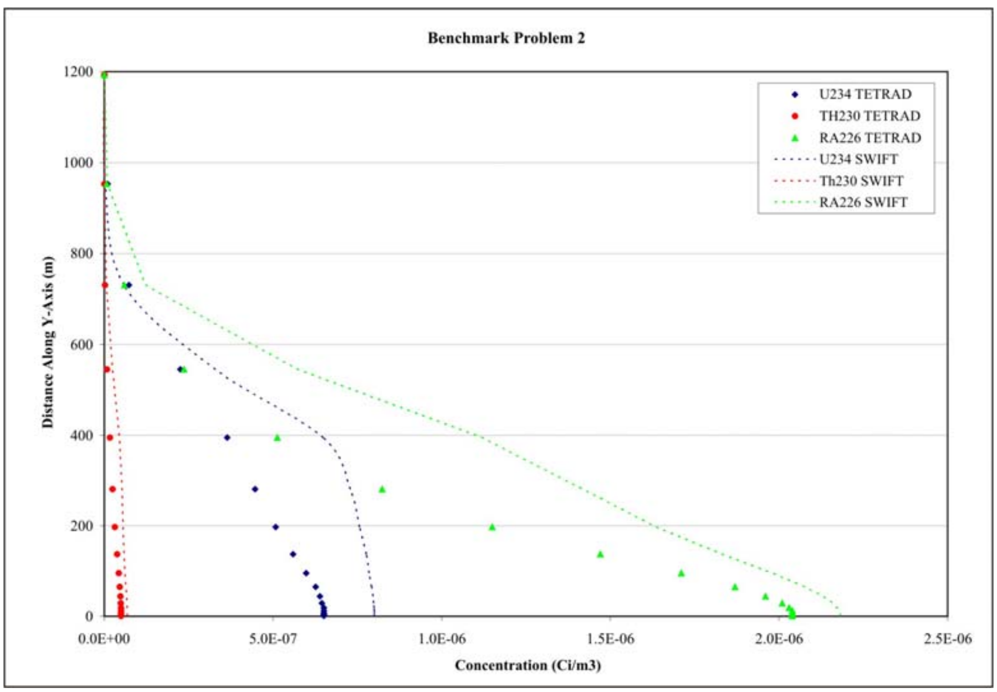

Figure 3.1. Comparison between TETRAD and SWIFT simulation results for Problem 2.

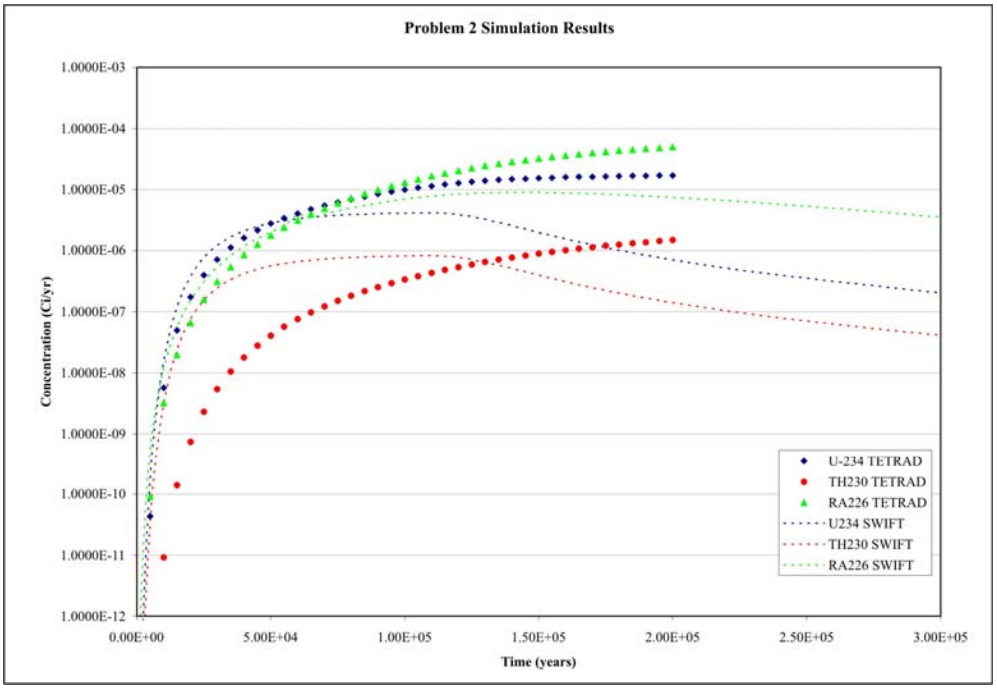

Figure 3.2. Comparison between TETRAD and SWIFT simulation results for Problem 2.

4 PROBLEM 3 - TRANSPORT WITH CHAIN DECAY IN FRACTURED POROUS MEDIA

4.1 PROBLEM STATEMENT AND OBJECTIVES

A summary of this problem including project description, assumptions, input specifications, and governing equations are presented in Ross et al. (1982). This problem corresponds to Problem 5 of INTRACOIN (1984) and Problem 9.1 of Ross et al. (1982).

As described in Ross et al. (1982), this problem is concerned with one-dimensional flow and transport of a three radionuclides decay chain in an aquifer consisting of porous blocks separated by a set of equally-spaced parallel fractures and confined above and below by impermeable beds. The objective of this simulation is to model the transport of a single three member decay chain that is released from storage over a specified period of time through a porous fractured aquifer. Assumptions include 1) groundwater flow occurs only in the fractures at a constant velocity, 2) the one-dimensional confined aquifer is semi-infinite, 3) fractures are planar and parallel to the groundwater flow direction, 4) convection and dispersion occur within the fractures only, 5) transport in the porous blocks is by molecular diffusion only, and 6) sorption is at equilibrium and occurs within the porous blocks only.

The problem was solved using the SWIFT numerical code. A description of the SWIFT code is presented in Section 2.1.

4.2 INPUT SPECIFICATIONS

This problem uses radionuclide inventory 2 presented in Table 2.2. Other input parameters, which are provided in Ross et al. (1982), are presented in Table 4.1.

Table 4.1. Input parameters for Problem 3.

Parameter	Value	Units
Release Duration	10^5	yr
Water velocity in fractures	500	m/yr
Dispersivity	50	m
Fracture spacing	5	m
Fracture width	10^{-4}	m
Nuclide diffusivity in pore water	2×10^{-10}	m^2/s
^{245}Cm retardation factor	570	
^{237}Np retardation factor	80	
^{233}U retardation factor	30	

Information on the SWIFT model discretization and other input parameters are provided in Ward et al. (1984).

4.3 COMPARISON OF RESULTS

Results of the SWIFT simulation for this problem are published in Ward et al. (1984). Results consisted of three points on the breakthrough curves of each radionuclide at an observation point located at a distance of 500 meters down-gradient from the source. These three points are the peak flux rate and the two half-maximum rates that occur before and after the peak. Concentration over time results were also provided for each radionuclide. GeoTrans (1988) compared the SWIFT results to results provided in the INTRACOIN (1984) report, and stated that the comparison was consistent.

INL provided TETRAD simulation results consisting of concentration over time for all three radionuclides. A copy of the INL simulation results for Problem 3 is provided in Attachment 1. These results were plotted against concentrations calculated by the SWIFT code. A comparison of these results is presented in Figure 4.1.

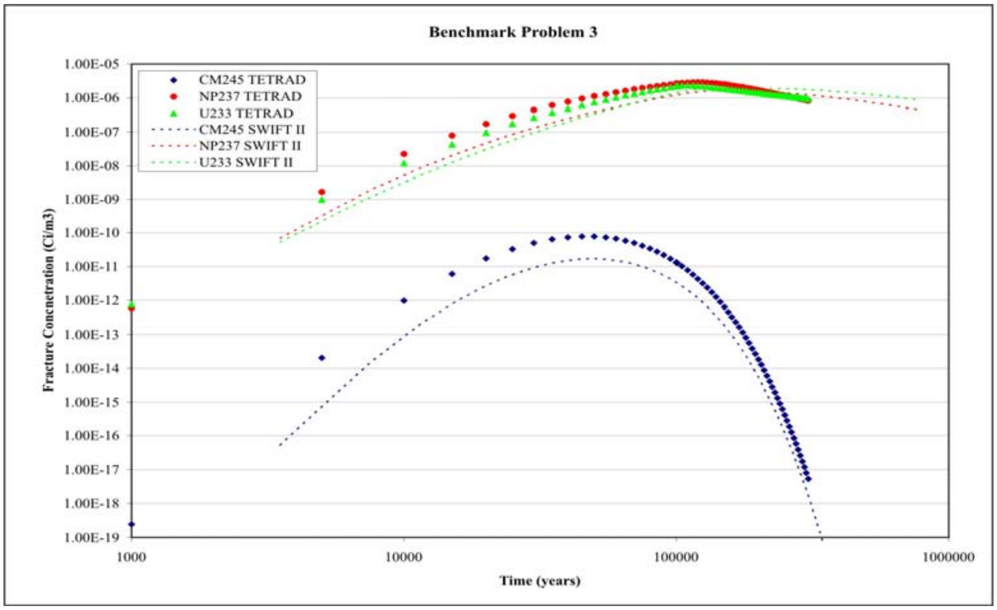

Figure 4.1. Comparison between TETRAD and SWIFT II simulation results for Problem 3.

5 PROBLEM 4 - HYDRODYNAMIC DISPERSION DURING ABSORPTION OF WATER BY SOIL

5.1 PROBLEM STATEMENT AND OBJECTIVES

A summary of this problem including project description, assumptions, input specifications, governing equations, and details on semi-analytical solutions is presented in Ross et al. (1982). This problem corresponds to Problem 4.1 for flow and Problem 10.1 for solute transport of Ross et al. (1982). A semi-analytical solution was developed by Philip (1955) for one-dimensional horizontal saturated flow. A solute transport semi-analytical solution was developed by Smiles et al. (1978).

As described in Ross et al. (1982), this problem considers solute transport in a semi-infinite horizontal tube of soil that is partially saturated with groundwater. The object is to determine the concentration field in a tube of soil that has uniform initial concentration and moisture content and in which the upstream boundary is subject to a prescribed moisture content and solute concentration. Transport processes include both advection and hydrodynamic dispersion, with both the hydraulic diffusivity and hydraulic dispersion being functions of moisture content.

The purpose of this problem is to verify the ability of a variably-saturated transport code to track a propagating wetting surface. Assumptions are 1) flow and transport are one-dimensional, 2) hydraulic and transport equation parameters such as porosity, saturated hydraulic conductivity, density, and cross-sectional area are constant, 3) transport processes include both advection, with the hydraulic diffusivity being a function of moisture content, 3) the hydrodynamic dispersion coefficient can be neglected, 4) no sorption of the solute occurs, and 5) the change in storage due to fluid compression is ignored.

This problem was solved using the Flow and Migration of Nonconservative Contaminants (FLAMINCO) code (GeoTrans, 1987). FLAMINCO is a three-dimensional finite element code that simulates fluid flow and transport of a single dissolved contaminant in saturated or variably-saturated porous media. The code can simulate advection, hydrodynamic dispersion, equilibrium adsorption transport processes and chemical degradation or radioactive decay.

5.2 INPUT SPECIFICATIONS

The input parameters, which are provided in Ross et al. (1982), are presented in Table 5.1. The initial uniform soil moisture content is 0.2 and the initial uniform solute concentration is 0.1 g/L. At t=0 the left boundary soil moisture content is raised to 0.45 (fully saturated) and the solute concentration to 1.0 g/L. The equations relating soil moisture, soil moisture diffusivity, relative permeability, and capillary pressure head are presented in Ross et al. (1982).

Table 5.1. Input Parameters for Problem 4.

Parameter	Value	Units
Soil effective porosity	0.45	
Hydraulic conductivity	1	cm/day
Tube length	20	cm
Residual saturation	0.333	
Initial pressure head	-83.33	cm
Molecular diffusion	1	cm^2/day

Information on the FLAMINCO model discretization and other input parameters is provided in GeoTrans (1987).

5.3 COMPARISON OF RESULTS

Results of the FLAMINCO simulation for solute transport are published graphically in GeoTrans (1987). Results were shown for solute concentration versus distance for three points in time (0.01, 0.06, and 0.11 days) and compared to the semi-analytical solution (Smiles et al., 1978). These FLAMINCO are comparable to the semi-analytical solution but offset slightly.

INL provided TETRAD simulation results for Problem 4 consisting of water saturation and solute concentration over time. A copy of the INL simulation results for Problem 4 is provided in Attachment 1. These results were plotted against water saturations and solute concentrations calculated by the appropriate semi-analytical solutions. A comparison of these results are presented in Figures 5.1 and 5.2. The flow (Figure 5.1) and transport (Figure 5.2) results are comparable to the semi-analytical solutions, although the solute concentrations are slightly offset from the calculated semi-analytical solution concentrations. The FLAMINCO report (GeoTrans, 1987) only graphically displayed the FLAMINCO data, so no direct comparison was made between the TETRAD and FLAMINCO results. Both data sets, however, were offset slightly from the calculated semi-analytical solution in the same direction and by the same apparent magnitude, indicating that results of these models are comparable.

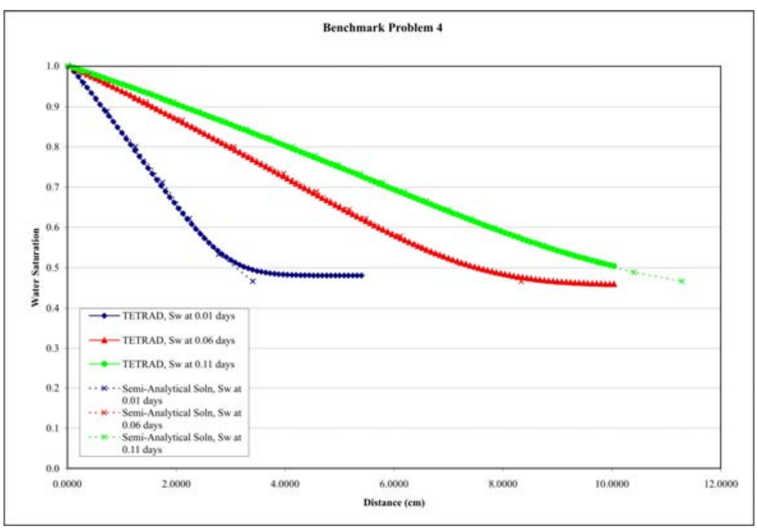

Figure 5.1. Comparison between TETRAD simulation results and semi-analytical solution for Problem 4.

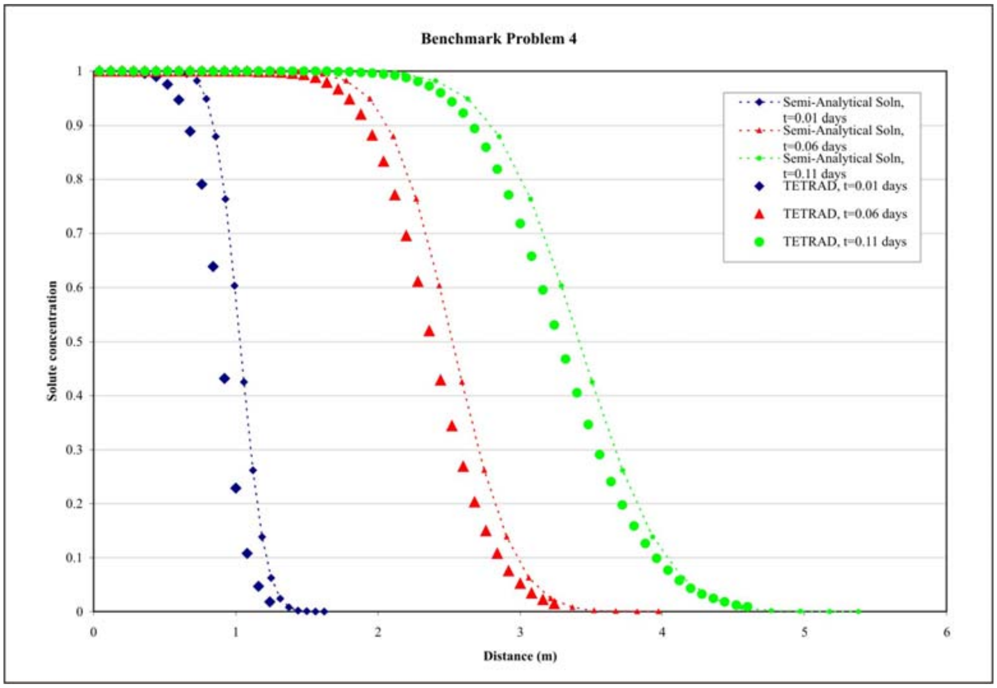

Figure 5.2. Comparison between TETRAD simulation results and semi-analytical solution for Problem 4.

6 PROBLEM 5 - FLOW AND SOLUTE TRANSPORT IN THE UNSATURATED ZONE

6.1 PROBLEM STATEMENT AND OBJECTIVES

A summary of this problem including project description, assumptions, input specifications, and governing equations are presented in Ross et al. (1982). This problem corresponds to Problem 4.2 for flow and Problem 10.2 for solute transport of Ross et al. (1982).

As described in Ross et al. (1982), this problem tests the capability of a variably saturated transport code to simulate two-dimensional non-conservative solute migration and concentration distributions in the unsaturated zone. The problem involves subjecting a certain portion of the model boundary to an increase in capillary pressure and solute concentration, which produces wetting and concentration fronts propagating through the medium with time.

Assumptions are 1) flow is two-dimensional, 2) transport is through advection, mechanical dispersion, and molecular diffusion, 3) adsorption is described by a linear equilibrium isotherm, 4) porosity, hydraulic conductivity, specific storage, and decay rate are constant, and 5) the rectangular model domain is partially saturated with uniform initial conditions.

This problem was simulated using the FLAMINCO code (GeoTrans, 1987). A description of the FLAMINCO code is provided in Section 5.1.

6.2 INPUT SPECIFICATIONS

The input parameters, which are provided in Ross et al. (1982), are presented in Table 6.1. The initial uniform soil moisture content is 0.2 and the initial uniform solute concentration is 0.1 g/L. At t=0 the capillary pressure and solute concentration along a certain portion of the left boundary are increased creating propagating moisture and concentration fronts through the soil medium with time. The equations relating soil moisture, soil moisture diffusivity, relative permeability, and capillary pressure head are presented in Ross et al. (1982).

Table 6.1. Input parameters for Problem 5.

Parameter	Value	Units
Soil effective porosity	0.45	
Hydraulic conductivity	1	cm/day
Rectangle length	15	cm
Rectangle width	10	cm
Initial pressure head	-90	cm
Longitudinal dispersivity	1	cm
Molecular diffusion	0.01	cm^2/day
Decay constant	0.001	d^{-1}
Retardation coefficient	2	

Information on the FLAMINCO model discretization and other input parameters are provided in GeoTrans (1987).

6.3 COMPARISON OF RESULTS

Results of the FLAMINCO simulation for solute transport are published in GeoTrans (1987). Results were provided for solute concentration versus distance in the x and y directions for three points in time (0.054, 0.165, and 0.508 days). The FLAMINCO results were compared to results from the FEMWASTE code. The results are comparable but the FLAMINCO results do not exhibit the oscillations that are present in the FEMWASTE results. The FEMWASTE results were compared to the results of the SATURN code (Huyakorn et al., 1983) and found to be comparable (GeoTrans, 1988).

INL provided TETRAD simulation results consisting of concentration over length and height. A copy of the INL simulation results for Problem 5 is provided in Attachment 1. These results were plotted against concentrations calculated by the FLAMINCO code. A comparison of these results is presented in Figures 6.1 and 6.2.

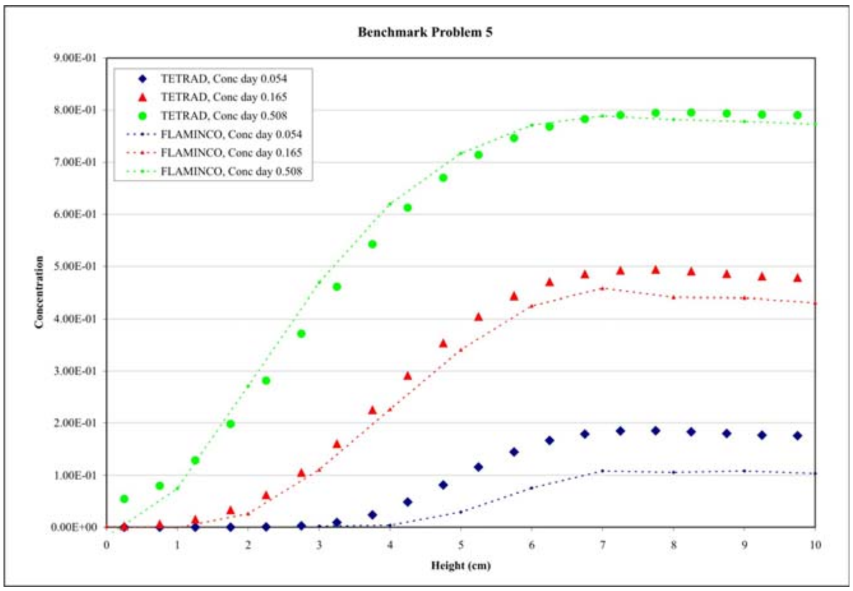

Figure 6.1. Comparison between TETRAD and FLAMINCO simulation results for Problem 5.

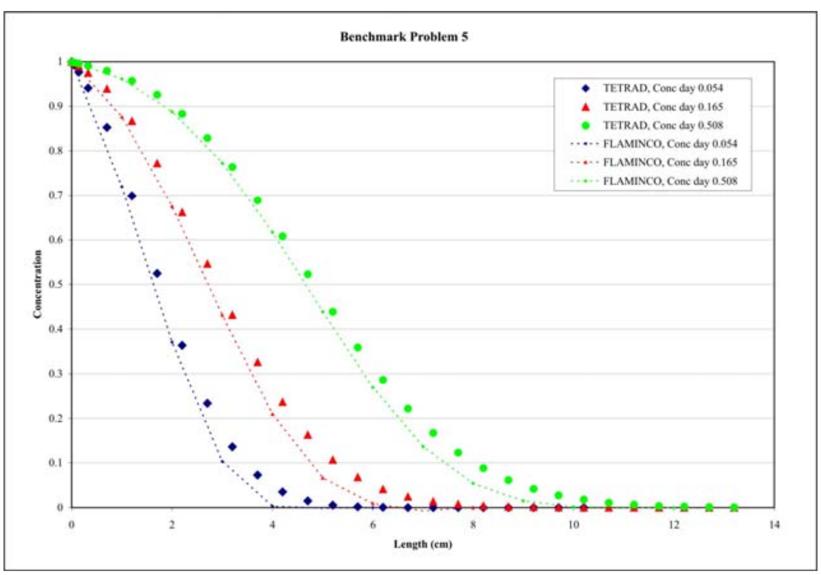

Figure 6.2. Comparison between TETRAD and FLAMINCO simulation results for Problem 5.

7 PROBLEM 6 - TRANSPORT OF INJECTATE IN A VARIABLY DIPPING AQUIFER

7.1 PROBLEM STATEMENT AND OBJECTIVES

A description of this problem is presented in DuPont (1999a). This problem was provided to DuPont by the United States Environmental Protection Agency (U.S. EPA) to reverify/revalidate DuPont's deep well injection model. This problem is referred to as EPA Case IId.

This problem involves the simulation of waste transport resulting from a fully penetrating injection well completed into an infinite reservoir with a variable dip, bounded above and below by impermeable beds. Only advective flow due to injection and fluid density differences, and dispersive flow are considered. No diffusive flow is considered. The objective of this simulation is to assess the ability of the model to predict pressure build-up and injected fluid transport (advective flow and hydrodynamic dispersion) in a variably-dipping two-dimensional aquifer. Assumptions include 1) the domain is an infinite uniform aquifer and is isotropic, 2) the injection well is fully penetrating, 3) only radial flow occurs during the injection period, 4) the background velocity is equal to zero, 5) molecular diffusion is negligible, and 6) the injected fluid has a different density than the aquifer fluid in order to drive advective flow after injection halts.

The problem was simulated using DuPont's deep well injection model and verified using the SWIFT code. A description of the SWIFT code is presented in Section 2.1.

7.2 INPUT SPECIFICATIONS

The reservoir dip is 0.5º from 5,000 feet down dip to 5,000 feet up dip from the injection well, changes to 0.75º from 5,000 to 15,000 feet up dip, then changes to 1.0º after 15,000 feet up dip of the well. Model input parameters are presented in Table 7.1.

Table 7.1. Input parameters for Problem 6.

Parameter	Value	Units
Reservoir permeability	750	md
Reservoir thickness	40	ft
Porosity	0.30	
Background velocity	0.0	ft/yr
Injectate density at reservoir conditions	62.4	lb/ft^3
Reservoir fluid density at reservoir conditions	66.144	
Injectate viscosity at reservoir conditions	0.413	cp
Reservoir fluid viscosity at reservoir conditions	0.583	cp
Reference pressure and temperature for fluids	2,325/155	psi/ºF
Water compressibility	$3.0x10^{-6}$	psi^{-1}
Rock compressibility	$3.0x10^{-6}$	psi^{-1}
Well radius	0.333	ft
Initial reservoir pressure	2,500	psi
Longitudinal dispersivity	100.0	ft
Transverse dispersivity	15.0	ft
Injection rate	500	gpm
Injection time	8	yr
Depth to center of injection interval of well	5,000	ft

Information on the DuPont model discretization and other input parameters is provided in DuPont (1999a).

7.3 COMPARISON OF RESULTS

Graphical results of the DuPont simulation are published in DuPont (1999a). Isoconcentration plots were provided for solute concentration reductions of 10^{-6} and 10^{-12}. Tabular results of plume dimensions were summarized in DuPont (2000). The DuPont simulation results were compared to results from SWIFT simulations conducted by U.S. EPA (Dupont, 2000) and GeoTrans (GeoTrans, 2000). The results are comparable with differences in plume dimensions ranging from 4 to 13% (DuPont, 2000).

INL provided TETRAD simulation results consisting of plots of normalized concentrations at 1, 5, 100, and 10,000 years. A copy of the INL simulation results for Problem 6 is provided in Attachment 1. From the concentration plots GeoTrans calculated plume dimensions based on the 10,000 year concentration plot. These results were compared to plume dimensions calculated by DuPont using their deep well injection model and the U.S. EPA using the SWIFT model. A summary of the plume dimensions is provided in Table 7.2.

Table 7.2. Dimensions of Simulated 10,000 Year Plume (Concentration = 10^{-12}) Measured from Injection Well for Problem 6.

Direction from Injection Well	TETRAD (feet)	EPA SWIFT (feet)	DuPont Model (feet)	Comparison to SWIFT	Comparison to DuPont
Length forward	18642	25588	22029	-27.1%	-15.4%
Length backward	6726	6232	5944	7.9%	13.2%
Total Length	25367	31820	27973	-20.3%	-9.3%
Lateral	6598	6704	5975	-1.6%	10.4%

A comparison of the TETRAD and DuPont deep well model 1, 5, 100, and 10,000 year plumes are presented in Figure 7.1.

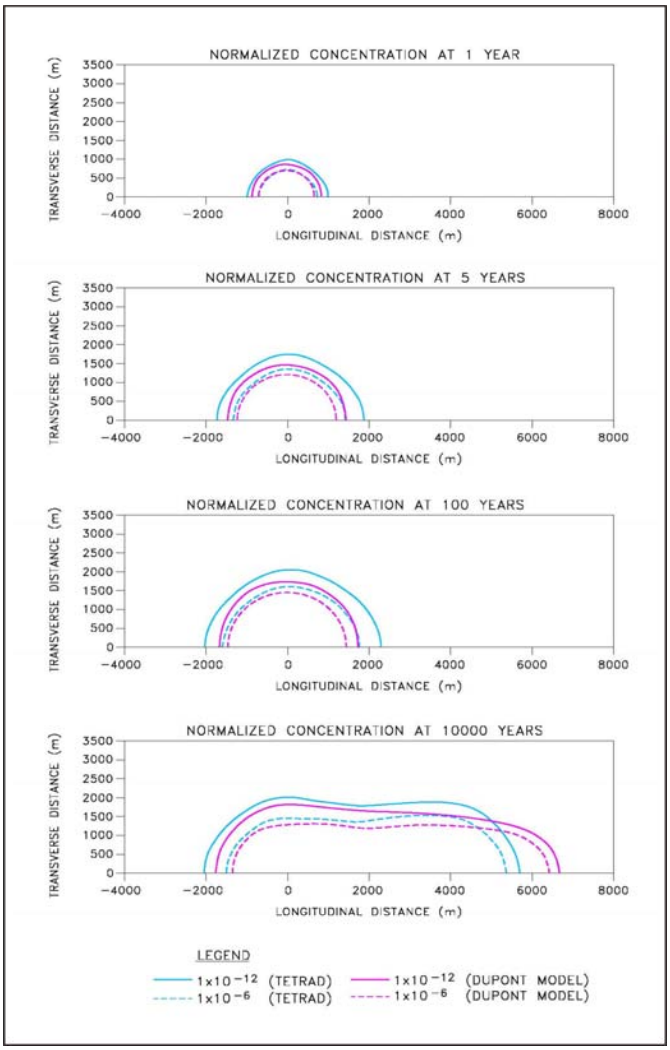

Figure 7.1. Comparison between TETRAD and DuPont Deep Well Model simulation results for Problem 6.

8 PROBLEM 7 – TRANSPORT OF INJECTATE IN A DIPPING AQUIFER WITH A BACKGROUND VELOCITY

8.1 PROBLEM STATEMENT AND OBJECTIVES

A description of this problem is presented in DuPont (1999b). This problem was provided to DuPont by the U.S. EPA to reverify/revalidate DuPont's deep well injection model. This problem is referred to as EPA Case IIf.

This problem is similar to EPA Case IId (Section 7.1) except that a constant background flow velocity and diffusive flow is added to the simulation, and the aquifer has a constant instead of a variable dip. This problem involves the calculation of waste transport resulting from a fully penetrating injection well completed into an infinite reservoir with a constant dip, bounded above and below by impermeable beds. The model simulates advective flow due to injection and fluid density differences, dispersive flow, and diffusive flow. The objective of this simulation is to assess the ability of the model to predict pressure build-up and injected fluid transport (advective flow and hydrodynamic dispersion) in a variably-dipping two-dimensional aquifer. Assumptions include1) the domain is an infinite uniform aquifer and is isotropic, 2) the injection well is fully penetrating, 3) only radial flow occurs during the injection period, 4) the background velocity is equal to 0.5 feet per year down dip, and 5) the injected fluid has a different viscosity than the aquifer fluid in order to drive advective flow after injection halts.

The problem was simulated using DuPont's deep well injection model and verified using the SWIFT code. A description of the SWIFT code is presented in Section 2.1.

8.2 INPUT SPECIFICATIONS

The reservoir has a constant dip of 1.5º. Model input parameters are presented in Table 8.1.

Table 8.1. Input parameters for Problem 7.

Parameter	Value	Units
Reservoir permeability	750	md
Reservoir thickness	40	ft
Porosity	0.30	
Background velocity	0.5	ft/yr
Injectate density at reservoir conditions	62.4	lb/ft^3
Reservoir fluid density at reservoir conditions	66.144	
Injectate viscosity at reservoir conditions	0.413	cp
Reservoir fluid viscosity at reservoir conditions	0.583	cp
Reference pressure and temperature for fluids	2,325/155	psi/ºF
Water compressibility	$3.0x10^{-6}$	psi^{-1}
Rock compressibility	$3.0x10^{-6}$	psi^{-1}
Well radius	0.333	ft
Initial reservoir pressure	2,500	psi
Longitudinal dispersivity	100.0	ft
Transverse dispersivity	15.0	ft
Free water molecular diffusivity	$4.3x10^{-3}$	ft^2/d
Injection rate	500	gpm
Injection time	8	yr
Depth to center of injection interval of well	5,000	ft

Information on the DuPont model discretization and other input parameters are provided in DuPont (1999b).

8.3 COMPARISON OF RESULTS

Graphical results of the DuPont simulation are published in DuPont (1999b). Isoconcentration plots were provided for solute concentration reductions of 10^{-6} and 10^{-12}. Tabular results of plume dimensions were summarized in DuPont (2000). The DuPont simulation results were compared to results from SWIFT simulations conducted by U.S. EPA (DuPont, 2000). The results are comparable with differences in plume dimension ranging from 4 to 13% (DuPont, 2000).

INL provided TETRAD simulation results consisting of plots of normalized concentrations at 1, 5, 100, and 10,000 years. A copy of the INL simulation results for Problem 7 is provided in Attachment 1. From the concentration plots GeoTrans calculated plume dimensions based on the 10,000 year concentration plot. These results were compared to plume dimensions calculated by DuPont using their deep well injection model and the U.S. EPA using the SWIFT model. A summary of the plume dimensions is provided in Table 8.2.

Table 8.2. Dimensions of Simulated 10,000 Year Plume (Concentration = 10^{-12}) Measured from Injection Well for Problem 7.

Direction from Injection Well	TETRAD (feet)	EPA SWIFT (feet)	DuPont Model (feet)	Comparison to SWIFT	Comparison to DuPont
Length forward	32349	34203	28813	-5.4%	12.3%
Length backward	10646	12141	13231	-12.3%	-19.5%
Total Length	42995	46344	42044	-7.2%	2.3%
Lateral	9442	7386	5875	27.8%	60.7%

A comparison of the TETRAD and DuPont deep well model 1, 5, 100, and 10,000 year plumes are presented in Figure 8.1.

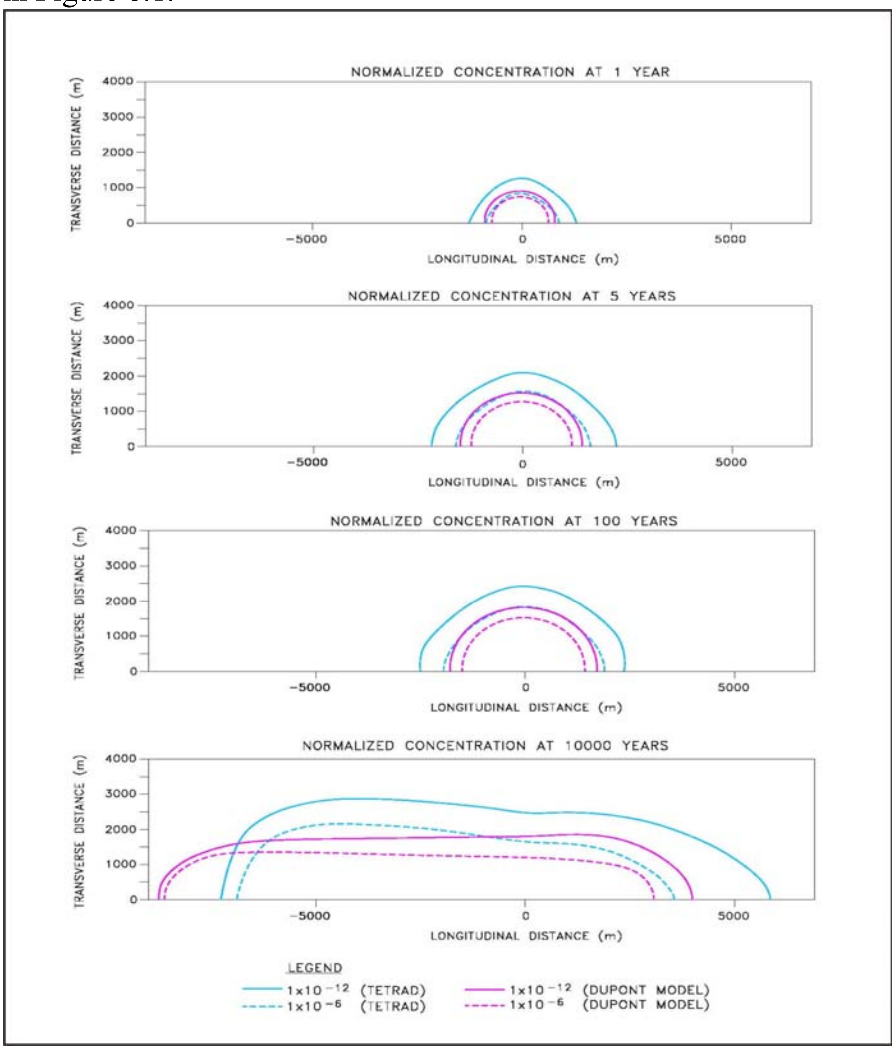

Figure 8.1. Comparison between TETRAD and DuPont Deep Well Model simulation results for Problem 7.

9 PROBLEM 8 - MULTIPHASE CARBON TETRACHLORIDE TRANSPORT IN UNSATURATED AND SATURATED MEDIA

9.1 PROBLEM STATEMENT AND OBJECTIVES

This benchmark problem was created by GeoTrans based on a comparison simulation (EX3DT) between TETRAD version 12.7 and 12.7ms presented in Appendix A of the Subsurface Flow and Transport Model Development for the Operable Unit 7-13/14 Remedial Investigation and Feasibility Study (Magnuson & Sondrup, 2006). This problem is analogous to environmental conditions as simulated in the OU 7-13/14 application.

This problem involves three-dimensional flow and transport of a carbon tetrachloride spill in saturated and unsaturated conditions. The model domain consists of a saturated and unsaturated soil unit and a non-continuous clay confining unit in the vadose zone. A spill of carbon tetrachloride is simulated in the sand unit near the top of the vadose zone above the clay unit. A gap in the clay unit down-gradient of the spill allows the carbon tetrachloride to migrate downward toward the saturated sand. After a time the spill is halted and the source area allowed to dissolve and migrate downward. A flooding event is also applied above the spill area for a period of time.

The objective of this problem is to test the ability of the TETRAD computer code to simulate the advection, dispersion, diffusion, adsorption, and decay of organic parameters in saturated and unsaturated environments. Assumptions include 1) flow and transport is three-dimensional, 2) a steady-state groundwater flow field and constant initial hydrogeologic parameters in the vadose and saturated zones, 3) equilibrium portioning between carbon tetrachloride phases, and 4) equilibrium sorption.

This benchmark problem was simulated using the T2VOC extension of the TOUGH2 code (Falta et al., 1995). T2VOC is a three-dimensional finite-difference numerical simulation program for modeling the transport of organic chemical contaminants in non-isothermal multiphase systems. T2VOC is based on the Transport of Unsaturated Groundwater and Heat (TOUGH2) code, which is a three-dimensional code for simulating the coupled transport of water, water vapor, air, and heat in porous and fractured porous media (Pruess, 1991).

9.2 INPUT SPECIFICATIONS

The three-dimensional domain consisted of the following discretization:

- 165 meters in the x-direction (19 columns); grid spacing = 13 columns of 5 m, 1 column of 10 m, 2 columns of 15 m, and 3 columns of 20 m.
- 165 meters in the y-direction (19 rows); grid spacing = 13 rows of 5 m, 1 rows of 10 m, 2 rows of 15 m, and 3 rows of 20 m.
- 61 meters in the z-direction (24 layers); layer spacing = 3 layers of 1 m, 4 layers of 2 m, 5 layers of 1 m, 1 layer of 2 m, 1 layer of 3 m, and 10 layers of 4 m.

The lithologic units consisted of a sand (material 1) with a clay (material 2) layer in layers 9, 10, and 11. There is a gap in the clay layer at columns 11, 12, 13, and 14.

The hydrogeologic properties used in the simulation are provided in Table 9.1.

Table 9.1. Hydrogeologic input parameters for Problem 8.

Parameter	Material 1 (Sand)	Material 2 (Clay)
Permeability, x-direction	$3.5x10^{-12}$ m^2 (3,500 mD)	$1.0x10^{-15}$ m^2 (1 mD)
Permeability, y-direction	$3.5x10^{-12}$ m^2 (3,500 mD)	$1.0x10^{-15}$ m^2 (1 mD)
Permeability, z-direction	$7.0x10^{-13}$ m^2 (700 mD)	$1.0x10^{-15}$ m^2 (1 mD)
Porosity	0.48	0.15
Residual Water Saturation	0.1	0.1
Residual NAPL Saturation	0.05	0.05
Residual Gas Saturation	0.001	0.001
Relative Permeability parameter, n	3	3
Sm, minimum wetting fluid saturation	0	0.36
Capillary pressure parameter, n (beta)	1.84	1.86
Alpha, gas-NAPL	10	10.8
Alpha, NAPL-water	11	6

Relative permeability is calculated based on a modified version of Stone's first three phase method (Stone, 1970). Capillary pressures are calculated based on three phase capillary functions from Parker et al. (1987). The values of the four relative permeability parameters used in the T2VOC model were arbitrarily selected but are generally realistic values. The values for the four capillary pressure parameters were taken from Parker et al. (1987) for sand and clay. Carbon tetrachloride properties were taken from Appendix A of Reid et al. (1987).

Surface background infiltration is 1 cm/year (0.02738 $kg/m^2/day$). A 4 meter head differential was applied from left to right across the simulation domain. On the left the water table was fixed at the top of Layer 20 and on the right at the top of Layer 21.

Carbon tetrachloride is injected in a single cell (column 8, row 1, layer 3) at a constant rate of $2.5x10^{-4}$ kg/sec (0.864 $kg/m^2/day$) for a period of one year (365 days). After one year carbon tetrachloride injection is halted, and a flooding event of increased recharge is applied to six grid cells (columns 7, 8, and 9; rows 1 and 2; layer 1) for a one year period. Infiltration at these six cells during this period is 7.9225x10-4 kg/sec (2.738 $kg/m^2/day$). At the end of the year of increased infiltration, the flooding event ends and normal background infiltration is applied across the entire model surface for a period of five years.

In summary, the transient model simulation consists of three events: 1) carbon tetrachloride injection and background infiltration for one year (day 0 to 365), 2) no VOC injection and increased infiltration at six grid cells, background infiltration at all other surface cells for one year (day 365 to 730), and 3) no VOC injection and background infiltration at all surface cells (day 730 to 2555).

9.3 COMPARISON OF RESULTS

After creating this three-dimensional problem, GeoTrans set up T2VOC input files and simulated the carbon tetrachloride plume at 365, 730, and 2555 days. GeoTrans also calculated the dissolved carbon tetrachloride concentration at five locations within the model domain:

- Location 1 – within the carbon tetrachloride source area,
- Location 2 – in the vadose zone just underneath the source area,
- Location 3 – in the vadose zone underneath the source area and just above the clay unit,
- Location 4 – in the vadose zone above the water table and underneath the gap in the clay unit, and
- Location 5 – at the water table near the down-gradient end of the model domain.

INL provided TETRAD simulation results consisting of carbon tetrachloride isoconcentration plots at 365, 730, and 2555 days at contour intervals of 0.1, 0.01, 0.001, and 0.0001 kg/m^3 and time series plots and tabulated data at location 1 to 5. A copy of the INL simulation results for Problem 8 is provided in Attachment 1. These results were plotted against concentrations calculated by the T2VOC code. A comparison of these results are presented in Figures 9.1 and 9.2.

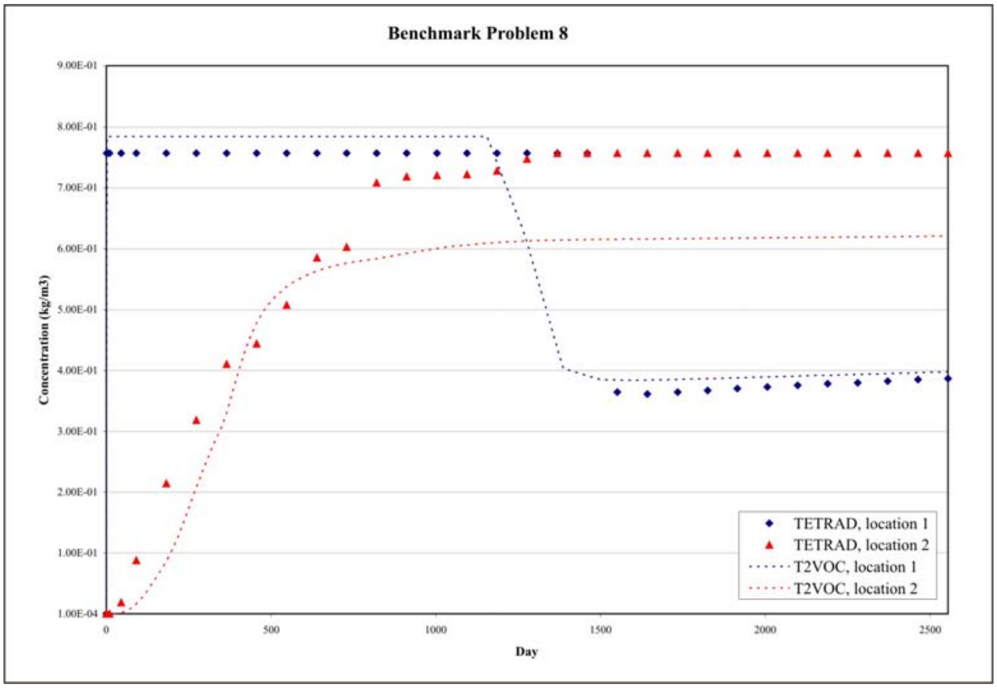

Figure 9.1. Comparison between TETRAD and T2VOC simulation results for Problem 8.

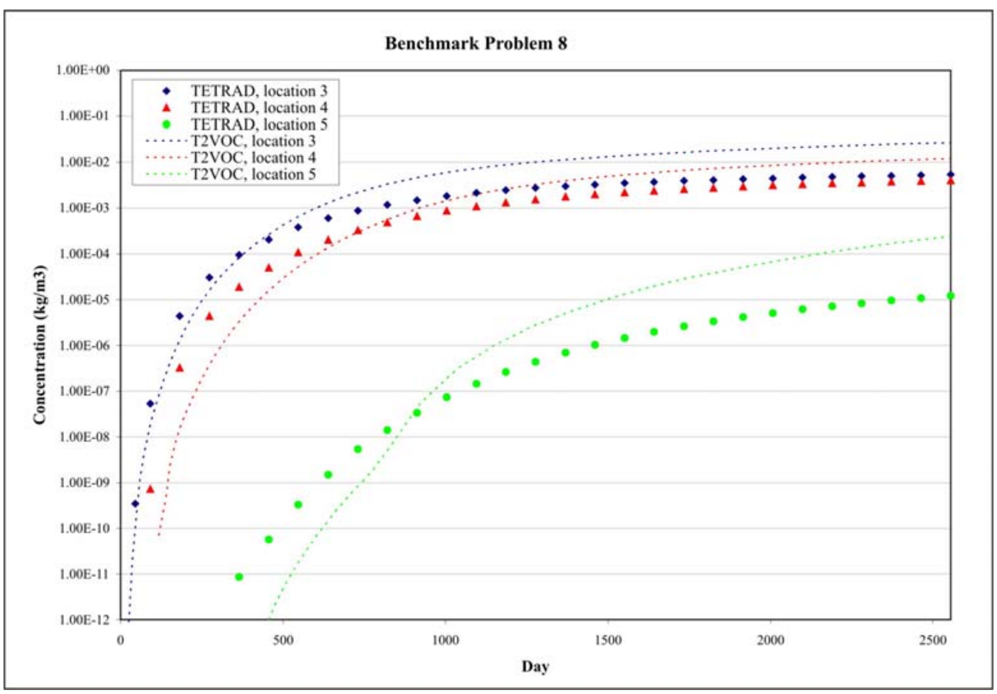

Figure 9.2. Comparison between TETRAD and T2VOC simulation results for Problem 8.

10 CONCLUSIONS AND RECOMMENDATIONS

The computer code TETRAD version 12.7ms has been tested with a set of eight benchmark problems that describe subsurface flow and transport processes characteristic of the setting of OU-7-13/14 at INL. This testing was conducted to provide objective verification of TETRAD for its application at OU-7-13/14. Verification demonstrates that a computer code properly simulates the processes it was designed to describe. It is one necessary step in assuring that an application is appropriate. The application most importantly depends upon assumptions and data used in its construction and validation (comparing observed data to model results). This benchmarking effort focuses on verification of TETRAD (its suitability for application at INL), but it does not address any specific application of TETRAD at INL.

The benchmark problems characterize the following processes and conditions:

- groundwater flow and radionuclide transport (advection, chain decay, and adsorption) in porous and fractured media in one and two dimensions;
- water flow and solute transport in the vadose zone in one and two dimensions;
- groundwater flow and solute transport affected by fluid density differences in two dimensions; and
- multiphase fluid flow (gas, water, nonaqueous phase liquid) and solute transport in three dimensions including gas phase diffusion and interphase transfer.

With the exception of the three-dimensional, multiphase problem, the test problems were selected from open technical literature or from problems used by U.S. EPA to test computer models used in permitting of injection wells for deep waste disposal.

The results of the TETRAD simulations for the selected benchmark problems compare well with those of other models. Exact comparisons are not expected due to several factors in code design and problem set up. The alternative computer models differ in details of the approximation of the governing partial differential equations, the treatment of nonlinear terms, and the solution of the resulting system of algebraic equations. To run a benchmark problem it is necessary to specify grid or element geometry, time stepping, and other numerical options that will affect the results. Many of these detailed numerical specifications were not available for the test problems.

The observable differences in results for the various models that have been tested illustrate the importance of documenting the sensitivity of a specific application, not only to its model data (such as, physical and chemical properties), but also to its numerical details. Results at low concentrations (relative to the source or solubility) can be very sensitive to grid spacing, time stepping, and convergence and weighting criteria. Where these low concentrations may be significant in an application, evaluation of the numerical specifications should be performed (whether the model used is TETRAD or another).

The TETRAD computer code has undergone numerous revisions since its original development. As new revisions are made to the code, it is recommended that each new version be benchmarked with the problems described here, in addition to revision-specific testing.

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ATTACHMENT 1

INL TETRAD SIMULATION BENCHMARKING REPORT DATED 9/13/06

VERIFICATION AND BENCHMARK TESTING OF THE TETRAD SIMULATOR, VERSION 12.7MS

1 INTRODUCTION AND SIMULATOR DESCRIPTION

GeoTrans, Inc., is conducting verification and benchmark testing of the TETRAD Version 12.7ms simulator to evaluate its correctness and operability for use as an environmental simulator. Verification is accomplished by comparing simple analytical solutions to those predicted by the simulator. The verification process has two main objectives. The first objective is to verify that the computational algorithms can accurately solve the governing equations and the second objective is to determine if the code is fully operational and no major programming errors persist. Benchmark testing involves comparing the simulator to another model, which has similar capabilities and has been widely accepted. The bench mark problems are generally more complex and realistic in nature than the verification problems. The objective of bench mark testing is to evaluate the simulators capabilities for solving problems of practical interest. The GeoTrans staff provided problem descriptions and the INL staff parameterized the problems with the TETRAD simulator. This report describes the TETRAD simulator, verification/benchmark problems, parameterization, and simulation results.

A description of the TETRAD simulator along with a description of each problem and discussion of how each problem was parameterized in TETRAD is presented in the following sections. The required output is provided in tables or graphical plots. The TETRAD input decks are provided in Appendix A of this report. A description of the electronic archive of the simulation input files, output files, and PV-Wave processing codes is provided in Appendix B.

1.1 TETRAD Simulator Description

The TETRAD simulator (Vinsome and Shook, 1993), Version 12.7ms is a robust, multiphase, multicomponent, and can also simulate dual porosity systems. TETRAD was originally developed as an enhanced oil recovery simulator for the petroleum industry. It has been successfully applied to simulate groundwater flow and transport at the INL Site for Waste Area Groups 1, 3, and 7. TETRAD has undergone limited verification and validation (Shook 1995) to demonstrate proficiency of the TETRAD simulator for use in modeling environmental fate and transport processes.

Modifications to improve the computation efficiency of the TETRAD, Version 12.7, simulator were described in Shook et al. (2003). The modified code resulting from that effort is called TETRAD, Version 12.7ms. Modifications were performed as part of an in-house laboratory-directed research and development project and consisted of allowing component specific convergence criteria to be specified. This allowed tighter convergence criteria on those components representing contaminants and looser criteria for those components representing pure water, air, and a required non aqueous phase liquid. Given the much larger mass of water and air present in the simulations, allowing appropriate convergence criteria for each component was a logical change.

1.1.1 Governing Equations

This section presents The TETRAD governing equations. The governing equations are presented to better elucidate the simulation approach needed to solve the verification and benchmark problem presented in this document. The general conservation equation solved by the TETRAD simulator for accumulation, flux, decay or degradation, and sources for any component i can be written as

$$\frac{\partial W_i}{\partial t} + \vec{\nabla} \cdot \vec{N_i} - R_i + q_i = 0 \qquad (1)$$

where

$\frac{\partial W_i}{\partial t}$ = is the accumulation term that consists of net changes in the concentration of the component i in any phase, including the adsorbed phase

$\nabla \bullet \vec{N}_i$ = is the flux of component i

R_i = the change in concentration arising from decay of component i

q_i represents sources or sinks of component i.

The accumulation term can be written as

$$W_i = \varphi(S_w \rho_w w_i + S_g \rho_g y_i + S_o \rho_o x_i) + ((1-\varphi)\rho_s V_i)/M_i \tag{2}$$

where

φ = the porosity

S_j = the phase saturations (w aqueous, g gaseous, o oleic)

ρ_j = the phase molar densities

w_i, y_i, and x_i = the mole fractions of i in the aqueous, gaseous, and oleic phases, respectively

ρ_s = the solid phase density

V_i = the mole fraction of i adsorbed on the solid phase

M_i = the molecular weight of i.

A generalized adsorption relationship is available in TETRAD that allows for adsorption onto the solid phase from any of the other three phases.

The flux term in Equation (1) is comprised of an advection and dispersion term for each phase given by

$$\vec{N}_i = [\rho_w \vec{u}_w w_i - \vec{D}_{iw} \cdot \vec{\nabla}(\rho_w w_i)] + [\rho_g \vec{u}_g y_g - \vec{D}_{ig} \cdot \vec{\nabla}(\rho_g y_i)] + [\rho_o \vec{u}_o x_i - \vec{D}_{io} \cdot \vec{\nabla}(\rho_o x_i)] \tag{3}$$

In Equation (3) the $\vec{u}_j$ are the phase advective fluxes, given by the multiphase version of Darcy's law:

$$\vec{u}_j = \frac{k k_{rj}}{\mu_j}(\vec{\nabla} P_j - \rho_j \vec{g}) \tag{4}$$

where

k = the intrinsic permeability

k_{rj} = the relative phase permeability

μ_j = the phase viscosity

P_j = the phase pressure

$\vec{g}$ = gravitational constant in vector form.

$\vec{D}_{ij}$ = the phase-dependant dispersion tensor comprised of molecular diffusion modified by porosity, phase saturation, tortuosity, and mechanical dispersion consisting of phase Dispersivity modified by directional components of advective phase fluxes (Bear 1972).

The reaction term in Equation (1) accounts for decay or degradation of component i and is written as:

$$R_i = -A_{i\varsigma}[m_j + V_i(1-\varphi)\rho_r] + A_{\omega i}[m_\omega + V_\omega(1-\varphi)\rho_r];\varsigma \neq \omega \tag{5}$$

where m_i is the total aqueous mass of i. The first term on the right hand side of Equation (5) accounts for i decaying with a rate constant $A_{i\varsigma}$ into component ς, whereas the second term on the right-hand side is the formation of i from destruction of component ω with a rate constant $A_{\omega i}$. The final term on the right-hand side in Equation (1) is the source/sink term, q_i. This term accounts for the addition or extraction of component i through wells or boundary conditions.

To solve the governing equations for variably saturated flow, TETRAD requires parameterization of saturation versus capillary pressure and saturation versus permeability for each lithologic material. These constitutive relationships can be parameterized with the van Genuchten (1980) equations, a Brooks-Corey type analytical function, or tabular input. TETRAD uses two-phase van Genuchten constitutive equations, as adapted by Parker et al. (1987) with slight modifications to the normalized saturation terms. The van Genuchten constitutive relations are:

$$\bar{S}_w = \frac{S_w - S_{wr}}{1 - S_{wr}}\ ; \quad \bar{S}_a = \frac{S_a}{1 - S_{wr}}; \quad \bar{S}_o = \frac{S_o}{1 - S_{wr}} \tag{6}$$

$$\bar{S}_L = \bar{S}_o + \bar{S}_w \tag{7}$$

$$P_{c\,ow} = \frac{\sigma_{ow}\,\rho_{fw}\,g}{\sigma_{aw}\alpha}\ [\,(\bar{S}_w)^{-1/\gamma} - 1]^{1/\beta} \tag{8}$$

$$P_{c\,ao} = \frac{\sigma_{ao}\rho_{fw}\,g}{\sigma_{aw}\alpha}\ [\,(1-\bar{S}_a)^{-1/\gamma} - 1]^{1/\beta} \tag{9}$$

$$P_{c\,aw} = P_{c\,ow} + P_{c\,ao} \tag{10}$$

$$k_{rw} = (\bar{S}_w)^{1/2}\ [1 - [1 - (\bar{S}_w)^{1/\gamma}\,]^{\gamma}]^2 \tag{11}$$

$$k_{ro} = (\bar{S}_o - \bar{S}_{or})^{1/2}\ [[1 - (\bar{S}_w)^{1/\gamma}\,]^{\gamma} - [1 - (\bar{S}_L)^{1/\gamma}\,]^{\gamma}]^2 \tag{12}$$

$$k_{ra} = (\bar{S}_a)^{1/2}\ [1 - (\bar{S}_L)^{1/\gamma}\,]^{2\gamma} \tag{13}$$

where

S_w = water saturation

S_o = oil saturation

S_a = air saturation

S_{wr} = residual water saturation

S_{or} = residual oil saturation

α = curve fitting parameter, related to inverse air entry potential (m^{-1},van Genuchten Alpha)

β = curve fitting parameter, affects nonlinearity of characteristic curve (van Genuchten n)

$\gamma = 1 - 1/\beta$

σ_{aw} = air-water interfacial tension (N/m)

σ_{ow} = oil-water interfacial tension (N/m)

σ_{ao} = air-oil interfacial tension (N/m)

ρ_{fw} = fresh water density (kg/m^3)

g = gravitational acceleration (m/s^2).

The Brooks-Corey type analytical formulas implemented in TETRAD are:

$$P_{c\,aw} = A_{aw}(1 - S_w)^{B_{aw}} \tag{14}$$

$$k_{ri} = A_i((S_i - S_{ir})/(1 - S_{ir}))^{B_i} \tag{15}$$

where

$P_{c\,aw}$ = capillary pressure between air and water (kPa)
k_{ri} = relative permeability of any phase i
S_i and S_{ir} = saturation and residual saturation of any phase i
A_{aw} (kPa), B_{aw}, A_i, and B_i = fitting parameters for the Brooks-Corey type functions.

1.1.2 TETRAD Attributes and Limitations for Environmental Simulation

Enhanced oil recovery (EOR) simulators used in the petroleum industry provide an attractive alternative to conventional simulators for environmental remediation studies because they can be applied to a greater variety of problems. The conventional dissolved phase contaminant fate and transport simulators solve the fluid mass and energy conservation equations separately from the transport conservation equations.

A single simulator that can solve conventional contaminant fate and transport problems, i.e. nitrate leaching from an unlined landfill or multiphase transport problems, i.e. LNAPL from waste oil disposal at the same landfill, would allow a single numerical model to be developed for a site with contamination for multiple sources. This is the case for the several superfund sites at the Idaho National Laboratory (INL) and this has prompted the INL to adopt the TETRAD petroleum/geothermal simulator for remediation studies

The draw back for using TETRAD to simulate very dilute solutes is that it is a compositional simulator and dissolved phase contaminants must be treated as a separate water component. For cases in which the contaminant concentration is very low, i.e. dissolved radionuclides at a few pCi/L, the contaminant mass must be scaled up (many orders of magnitude) to a reasonable mass fraction for maintaining mass balance. The problem is further compounded when simulating reacting contaminants, which result in mass transfer from solution to the porous media. When contaminants are placed into the model or are sorbed onto the porous media, they represent a volume that increases or decreases the total amount of water in the system. This gain or loss of volume may change the pressure field. The contaminants must be scaled up sufficiently to maintain proper mass balance, while still maintaining a small enough mass fraction as to not affect the water pressure.

2 PROBLEM 8.1: ONE-DIMENSIONAL TRANSPORT WITH CHAIN DECAY

2.1 Problem Description and Objectives

This problem simulates one-dimensional transport away from a river channel with a three chain radionuclide source. The aquifer is assumed to be infinite with a constant velocity. The source undergoes decay as a three chain series. The problem includes two decay chains with 3 sets of retardation values and 3 dispersivity values each (0m, 50m, and 500m). This problem requires 18 simulations to include all possible combinations. The source period is 100,000 years.The aquifer linear velocity is prescribed to be 1 m/year. The product of the aquifer velocity, porosity, source duration, and river cross sectional is assumed to be 1. This results in the river concentration being the same as the aquifer boundary concentration. Table 1 contains the simulated nuclides, half-lives, inventory, and retardation values. The test assumptions include:

- Flow and transport is one-dimensional.
- Velocity is constant.
- The domain is semi-infinite.
- Equilibrium sorption.

The objective of this problem is to test a the simulation code with transport conditions including large and small Peclet numbers and conditions of decay daughters moving much faster or slower than the parent. The required output is the concentration through time at a location 500 m down gradient of the source.

Table 1. Problem 8.1 simulated radionuclides.

Nuclide	Half-Life (yr)	Specific Activity (Ci/g)	Initial Inventory Concentration (Ci/m^3)	Retardation Set 1 Values	Retardation Set 2 Values	Retardation Set 3 Values
Decay Chain 1						
U-234	2.445e+5	6.2e-3	1.0	300	60	30
Th-230	7.7e+4	1.9e-2	0.01	20,000	500	2,300
Ra-226	1.6e+3	1.0e+0	0.004	10,000	20	1,100
Decay Chain 2						
Cm-245	8.5e+3	1.0e-1	0.7	5,000	60	570
Np-237	2.14e+6	6.9e-4	1.0	700	200	80
U-233	1.592e+5	9.5e-3	0.004	300	60	30

2.2 TETRAD Simulation

The simulation grid was 10,000 m using 251 grid blocks of 40 m each. The parameterization approach used with the TETRAD simulator was set the initial concentration and pressure at the up gradient boundary grid block and to increase the volume of the grid block by a factor of 1.e+10. This allows a constant pressure and concentration boundary condition throughout the simulation. The nuclides within the source grid block were allowed to decay and ingrow through time. The grid block volume multiplication is accomplished with the TETRAD ‘BVMULT’ keyword. The ‘AQUIFER’ keyword for setting a constant pressure or concentration boundary condition could not be used because the boundary condition concentration must change through time as decay and ingrowth occur. The rock density within the source block was set to zero to prevent sorption within the source area. The down gradient boundary condition used the ‘AQUIFER’ and ‘SSTATE’ keywords to set a Dirichlet boundary condition. The source grid block was assumed to be outside of the solution domain.

Boundary pressure, porosity, and permeability values were chosen to provide a 1m/year linear velocity. The linear pressure gradient was initialized in the simulator by specifying an initial pressure in each grid block in equilibrium with the boundary conditions. The source was turned after 1e+5 years by using the 'TMULT' keyword to set the source grid block transmissibility to 0 and placing a new 'AQUIFER' keyword pressure boundary on the model grid block adjacent to the former source grid block.

Dispersion control was implemented within the TETRAD simulator by specifying a second order accurate in space solution using the 'DISCW' keyword. The liquid viscosity was calculated internally within the TETRAD simulator using the Gottfried temperature relationship.Table 2 summarizes the TETRAD simulation parameters. The TETRAD sorption coefficient (K_d) values were calculated from the radionuclide retardation factor (R_d), the soil's bulk density (ρ_b), and moisture content (θ) from the equation

$$R_d = 1 + \frac{\rho_b K_d}{\theta}. \tag{16}$$

The TETRAD simulator requires the radionuclides by simulated in mass concentration instead of activity concentration. This is required to conserve total mass in the parent to daughter decay process. simulation in activity concentrations would result in more or less daughter product than the parent decay, if the daughter half-life was different from the parent. The river channel activity concentrations were converted to mass concentrations before input into the model and converted back to activity concentration during the post-processing of the simulation results. Table 1 contains the nuclide specific activities used in the concentration conversion.

TETRAD is a purely compositional simulator and requires dissolved phase contaminants to be treated as a separate water component in the aqueous phase with finite mass and volume. For cases in which the contaminant concentration is very low, i.e. dissolved radionuclides at a few pCi/L, the contaminant mass must be scaled up many orders of magnitude to a "reasonable" mass fraction in order to balance mass. When aqueous phase (dissolved) contaminants are initially placed into the model or are sorbed onto the porous media, they represent a finite volume of groundwater that increases or decreases the total amount of water in the system. This gain or loss of volume may change the water pressure field, if the scaling factor is too large. The contaminants must be scaled up sufficiently to maintain proper mass balance, while still maintaining a small enough mass fraction as to not affect the water pressure.The scaling factor used in this simulation was 1 Ci/L corresponds to 1.e-9 mole fraction. This concentration resulted in essentially no change in the pressure field as the solute front progressed.

The simulation results are as expected. Greater dispersivity values result in greater solute spreading and a more diffuse breakthrough. No numerical problems were encountered and the tracer mass balance was excellent with a relative error of 1e-15 magnitude. Figure 1 illustrates the concentration vs. distance for the inventory 1, retardation set 1, and 0 m dispersivity simulation. Figure 2 illustrates the concentration vs. distance for the inventory 2, retardation set 1, and 0 m dispersivity simulation. The required concentration history at 500 m down gradient for the inventory 1 simulations are provided in Table 3. Table 4 contains the concentration history for the inventory 2 simulations.

Table 2. TETRAD simulation parameters for problem 8.1.

Parameter	Value
Porosity	0.5
Perrmeability (mD)	192.45
Liquid Density (Kg/m^3)	1000
Viscosity (mPa S)	1.17
Temperature (degree C)	20.

Parameter	Value
Particle Density (Kg/m^3)	2650.
Pressure Head Gradient (m/m)	0.01
Pore Space Compressibility (1/KPa)	1.5e-7

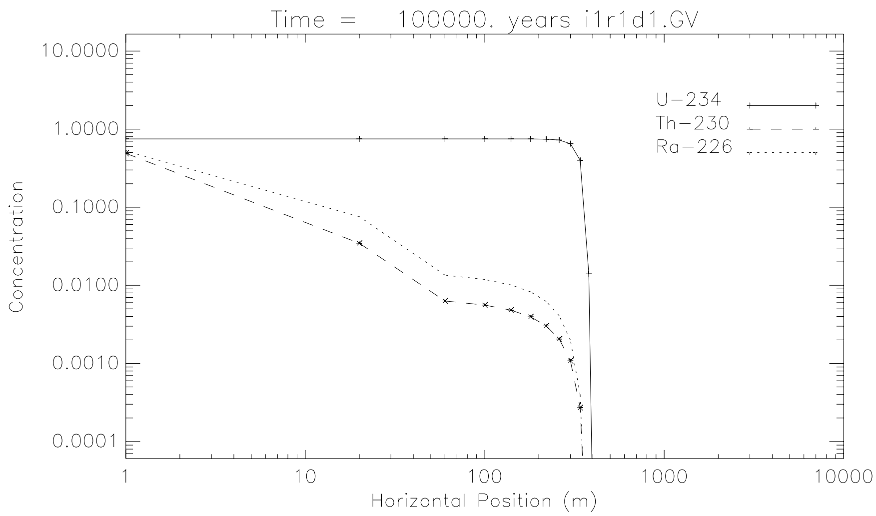

Figure 1. Concentration vs. distance for the inventory 1, retardation set 1, and 0 m dispersivity simulation of problem 8.1.

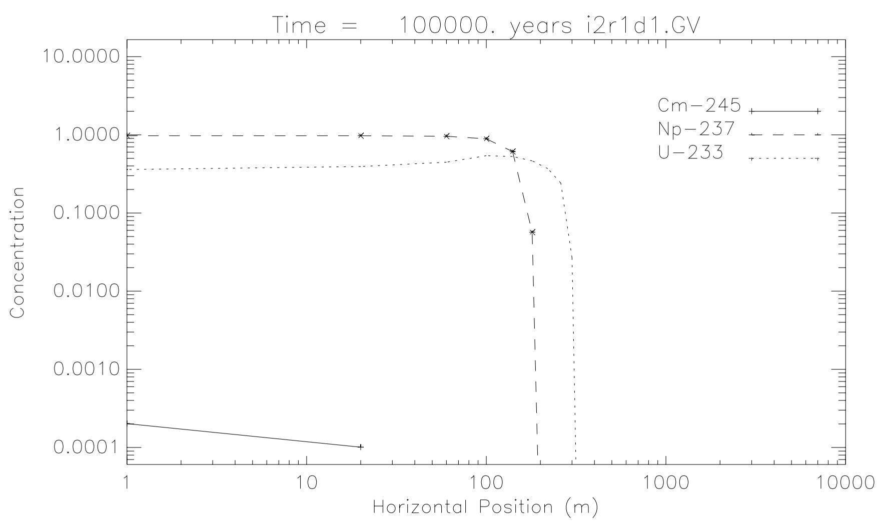

Figure 2. Concentration vs. distance for the inventory 2, retardation set 1, and 0 m dispersivity simulation of problem 8.1

Table 3. Concentration history at 500 m for the inventory one (U-234, Th-230, Ra-226) simulations of problem 8.1.

Time (yr)	U-234 (Ci/m^3)	Th-230 (Ci/m^3)	Ra-226 (Ci/m^3)
Retardation Set 1and 0m Dispersivity, Output File=i1r1d1.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.000000	0.000000	0.000000
20000.0	0.000000	0.000000	0.000000
30000.0	0.000000	0.000000	0.000000
40000.0	0.000000	0.000000	0.000000
50000.0	0.000000	0.000000	0.000000
60000.0	0.000000	0.000000	0.000000
70000.0	0.000000	0.000000	0.000000
80000.0	0.000000	0.000000	0.000000
90000.0	0.000000	0.000000	0.000000
100000.	0.000000	0.000000	0.000000
110000.	0.000000	0.000000	0.000000
120000.	0.000000	0.000000	0.000000
130000.	5.37540e-008	2.77400e-011	3.56000e-011
140000.	0.0948600	2.79300e-005	2.76000e-005
150000.	0.407340	0.000347700	0.000544000
160000.	0.546840	0.000934800	0.00173000
170000.	0.585900	0.00157510	0.00311000
180000.	0.589000	0.00218500	0.00445000
190000.	0.579700	0.00273600	0.00567000
200000.	0.565440	0.00321100	0.00675000
210000.	0.550560	0.00364800	0.00770000
220000.	0.535060	0.00400900	0.00853000
230000.	0.520180	0.00433200	0.00925000
240000.	0.424700	0.00457900	0.00984000
250000.	0.182900	0.00456000	0.00993000
260000.	0.0706800	0.00431300	0.00948000
270000.	0.0279000	0.00399000	0.00881000
280000.	0.0112220	0.00366700	0.00811000
290000.	0.00456320	0.00336300	0.00743000
300000.	0.00187860	0.00305900	0.00679000
Retardation Set 2 and 0m Dispersivity, Output File=i1r2d1.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.000000	0.000000	0.000000
20000.0	0.000000	0.000000	0.00770000
30000.0	0.576600	0.000845500	0.141000
40000.0	0.886600	0.0101460	0.407000
50000.0	0.868000	0.0190000	0.653000

Time (yr)	U-234 (Ci/m^3)	Th-230 (Ci/m^3)	Ra-226 (Ci/m^3)
60000.0	0.843200	0.0269800	0.870000
70000.0	0.818400	0.0338200	1.07000
80000.0	0.793600	0.0397100	1.25000
90000.0	0.775000	0.0448400	1.41000
100000.	0.750200	0.0492100	1.56000
110000.	0.731600	0.0530100	1.69000
120000.	0.713000	0.0560500	1.80000
130000.	0.256680	0.0581400	1.79000
140000.	0.00295120	0.0533900	1.69000
150000.	4.28420e-005	0.0482600	1.58000
160000.	6.44800e-007	0.0437000	1.51000
170000.	9.67200e-009	0.0397100	1.42000
180000.	1.45700e-010	0.0357200	1.38000
190000.	2.19480e-012	0.0321100	1.35000
200000.	3.31080e-014	0.0290700	1.30000
210000.	4.97860e-016	0.0262200	1.30000
220000.	7.50200e-018	0.0239400	1.27000
230000.	1.13460e-019	0.0218500	1.27000
240000.	1.71120e-021	0.0199500	1.25000
250000.	2.58540e-023	0.0181830	1.26000
260000.	3.89360e-025	0.0180690	1.22000
270000.	5.87140e-027	0.0277400	1.20000
280000.	8.86600e-029	0.0400900	1.12000
290000.	0.000000	0.0448400	1.06000
300000.	0.000000	0.0446500	0.926000
Retardation Set 3 and 0m Dispersivity, Output File=i1r3d1.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.000000	0.000000	0.000000
20000.0	0.942400	0.000537700	0.000753000
30000.0	0.917600	0.00151050	0.00297000
40000.0	0.892800	0.00237500	0.00498000
50000.0	0.868000	0.00313500	0.00677000
60000.0	0.843200	0.00380000	0.00833000
70000.0	0.818400	0.00437000	0.00970000
80000.0	0.793600	0.00488300	0.0109000
90000.0	0.775000	0.00532000	0.0119000
100000.	0.750200	0.00568100	0.0128000
110000.	0.731600	0.00600400	0.0136000
120000.	0.00313100	0.00587100	0.0137000
130000.	7.00600e-007	0.00535800	0.0125000
140000.	1.63060e-010	0.00490200	0.0114000
150000.	3.78820e-014	0.00446500	0.0104000

Time (yr)	U-234 (Ci/m^3)	Th-230 (Ci/m^3)	Ra-226 (Ci/m^3)
160000.	8.80400e-018	0.00408500	0.00953000
170000.	2.03980e-021	0.00372400	0.00870000
180000.	4.77400e-025	0.00340100	0.00792000
190000.	1.12840e-028	0.00311600	0.00723000
200000.	0.000000	0.00283100	0.00661000
210000.	0.000000	0.00258400	0.00603000
220000.	0.000000	0.00237500	0.00552000
230000.	0.000000	0.00216600	0.00505000
240000.	0.000000	0.00197600	0.00461000
250000.	0.000000	0.00180310	0.00420000
260000.	0.000000	0.00164730	0.00383000
270000.	0.000000	0.00150290	0.00350000
280000.	0.000000	0.00137370	0.00320000
290000.	0.000000	0.00125400	0.00291000
300000.	0.000000	0.00114570	0.00265000
Retardation Set 1 and 50m Dispersivity, Output File=i1r1d2.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	9.23800e-011	9.86100e-015	5.50000e-015
20000.0	2.12040e-007	4.73100e-011	4.35000e-011
30000.0	1.31440e-005	4.71200e-009	5.54000e-009
40000.0	0.000187240	9.55700e-008	1.31000e-007
50000.0	0.00120280	8.22700e-007	1.25000e-006
60000.0	0.00474300	4.16100e-006	6.79000e-006
70000.0	0.0133920	1.46680e-005	2.53000e-005
80000.0	0.0300080	4.00900e-005	7.19000e-005
90000.0	0.0562960	9.02500e-005	0.000167000
100000.	0.0923800	0.000175750	0.000335000
110000.	0.137020	0.000305900	0.000594000
120000.	0.186620	0.000482600	0.000956000
130000.	0.238700	0.000710600	0.00143000
140000.	0.291400	0.000984200	0.00200000
150000.	0.338520	0.00129770	0.00266000
160000.	0.372000	0.00163400	0.00338000
170000.	0.389980	0.00197600	0.00412000
180000.	0.391840	0.00229900	0.00484000
190000.	0.381920	0.00258400	0.00548000
200000.	0.363940	0.00283100	0.00604000
210000.	0.342240	0.00304000	0.00649000
220000.	0.311860	0.00319200	0.00684000
230000.	0.277760	0.00328700	0.00708000
240000.	0.241180	0.00332500	0.00719000
250000.	0.205220	0.00330600	0.00720000

Time (yr)	U-234 (Ci/m^3)	Th-230 (Ci/m^3)	Ra-226 (Ci/m^3)
260000.	0.171740	0.00326800	0.00711000
270000.	0.142600	0.00317300	0.00694000
280000.	0.117800	0.00305900	0.00671000
290000.	0.0961000	0.00292600	0.00643000
300000.	0.0787400	0.00279300	0.00612000
Retardation Set 2 and 50m Dispersivity, Output File=i1r2d2.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.00146320	1.89810e-006	0.00314000
20000.0	0.117180	0.000427500	0.0496000
30000.0	0.468720	0.00364800	0.193000
40000.0	0.706800	0.0101270	0.411000
50000.0	0.799800	0.0177840	0.653000
60000.0	0.818400	0.0252700	0.892000
70000.0	0.812200	0.0321100	1.12000
80000.0	0.793600	0.0381900	1.33000
90000.0	0.775000	0.0435100	1.54000
100000.	0.750200	0.0480700	1.73000
110000.	0.731600	0.0522500	1.88000
120000.	0.617520	0.0554800	1.97000
130000.	0.337900	0.0564300	1.97000
140000.	0.141360	0.0547200	1.92000
150000.	0.0533820	0.0518700	1.84000
160000.	0.0192200	0.0492100	1.76000
170000.	0.00675800	0.0471200	1.68000
180000.	0.00232500	0.0456000	1.60000
190000.	0.000799800	0.0446500	1.51000
200000.	0.000272800	0.0440800	1.41000
210000.	9.30000e-005	0.0437000	1.31000
220000.	3.18060e-005	0.0429400	1.21000
230000.	1.08500e-005	0.0414200	1.11000
240000.	3.70140e-006	0.0393300	1.00000
250000.	1.26480e-006	0.0366700	0.905000
260000.	4.32760e-007	0.0338200	0.805000
270000.	1.48180e-007	0.0307800	0.710000
280000.	5.09020e-008	0.0279300	0.623000
290000.	1.74840e-008	0.0250800	0.542000
300000.	6.01400e-009	0.0224200	0.469000
Retardation Set 3 and 50m Dispersivity, Output File=i1r3d2.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.121520	2.20400e-005	1.93000e-005
20000.0	0.750200	0.000537700	0.000865000
30000.0	0.892800	0.00141740	0.00277000

Time (yr)	U-234 (Ci/m^3)	Th-230 (Ci/m^3)	Ra-226 (Ci/m^3)
40000.0	0.886600	0.00228000	0.00474000
50000.0	0.868000	0.00304000	0.00652000
60000.0	0.843200	0.00370500	0.00809000
70000.0	0.818400	0.00429400	0.00946000
80000.0	0.793600	0.00480700	0.0107000
90000.0	0.775000	0.00524400	0.0117000
100000.	0.750200	0.00562400	0.0126000
110000.	0.632400	0.00592800	0.0133000
120000.	0.150040	0.00581400	0.0133000
130000.	0.0210800	0.00539600	0.0124000
140000.	0.00262880	0.00492100	0.0114000
150000.	0.000317440	0.00450300	0.0104000
160000.	3.80060e-005	0.00410400	0.00952000
170000.	4.55700e-006	0.00376200	0.00869000
180000.	5.48080e-007	0.00342000	0.00794000
190000.	6.63400e-008	0.00313500	0.00725000
200000.	8.06000e-009	0.00285000	0.00662000
210000.	9.85800e-010	0.00260300	0.00604000
220000.	1.20900e-010	0.00237500	0.00551000
230000.	1.49420e-011	0.00216600	0.00504000
240000.	1.84760e-012	0.00199500	0.00460000
250000.	2.30020e-013	0.00181450	0.00420000
260000.	2.87680e-014	0.00165680	0.00384000
270000.	3.60220e-015	0.00151430	0.00351000
280000.	4.52600e-016	0.00138320	0.00320000
290000.	5.70400e-017	0.00126540	0.00293000
300000.	7.19200e-018	0.00115710	0.00268000
Retardation Set 1 and 500 m Dispersivity, Output File=i1r1d3.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.00107260	2.31800e-007	2.00000e-007
20000.0	0.0140120	8.22700e-006	1.16000e-005
30000.0	0.0390600	4.04700e-005	6.82000e-005
40000.0	0.0688200	0.000105260	0.000193000
50000.0	0.0992000	0.000203300	0.000389000
60000.0	0.128340	0.000328700	0.000650000
70000.0	0.154380	0.000478800	0.000965000
80000.0	0.178560	0.000647900	0.00132000
90000.0	0.199640	0.000832200	0.00171000
100000.	0.218240	0.00102220	0.00213000
110000.	0.233740	0.00121980	0.00255000
120000.	0.238080	0.00141360	0.00297000
130000.	0.230640	0.00158650	0.00336000

Time (yr)	U-234 (Ci/m^3)	Th-230 (Ci/m^3)	Ra-226 (Ci/m^3)
140000.	0.218240	0.00173280	0.00369000
150000.	0.203980	0.00184870	0.00396000
160000.	0.188480	0.00193800	0.00416000
170000.	0.174220	0.00199500	0.00430000
180000.	0.160580	0.00203300	0.00440000
190000.	0.148180	0.00205200	0.00444000
200000.	0.136400	0.00205200	0.00446000
210000.	0.125860	0.00203300	0.00443000
220000.	0.115940	0.00201400	0.00438000
230000.	0.107260	0.00197600	0.00431000
240000.	0.0985800	0.00193800	0.00423000
250000.	0.0911400	0.00188860	0.00412000
260000.	0.0843200	0.00183540	0.00401000
270000.	0.0781200	0.00177840	0.00389000
280000.	0.0725400	0.00171950	0.00376000
290000.	0.0669600	0.00165680	0.00363000
300000.	0.0620000	0.00159410	0.00349000
Retardation Set 2and 500m Dispersivity, Output File=i1r2d3.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.110980	0.000435100	0.0269000
20000.0	0.273420	0.00269800	0.127000
30000.0	0.391220	0.00665000	0.283000
40000.0	0.473060	0.0119890	0.479000
50000.0	0.530100	0.0183730	0.700000
60000.0	0.569160	0.0254600	0.938000
70000.0	0.595820	0.0332500	1.18000
80000.0	0.612560	0.0412300	1.43000
90000.0	0.620000	0.0492100	1.67000
100000.	0.626200	0.0571900	1.90000
110000.	0.541880	0.0646000	1.95000
120000.	0.416640	0.0693500	1.92000
130000.	0.322400	0.0704900	1.84000
140000.	0.252960	0.0687800	1.73000
150000.	0.200880	0.0653600	1.60000
160000.	0.161200	0.0609900	1.48000
170000.	0.130820	0.0562400	1.35000
180000.	0.106640	0.0514900	1.23000
190000.	0.0874200	0.0469300	1.12000
200000.	0.0719200	0.0425600	1.02000
210000.	0.0597060	0.0385700	0.919000
220000.	0.0496620	0.0347700	0.830000
230000.	0.0414780	0.0313500	0.749000

Time (yr)	U-234 (Ci/m^3)	Th-230 (Ci/m^3)	Ra-226 (Ci/m^3)
240000.	0.0347200	0.0283100	0.675000
250000.	0.0291400	0.0254600	0.608000
260000.	0.0245520	0.0228000	0.548000
270000.	0.0207080	0.0205200	0.493000
280000.	0.0175460	0.0184490	0.443000
290000.	0.0148180	0.0165680	0.399000
300000.	0.0125860	0.0148770	0.358000
Retardation Set 3 and 500 m Dispersivity, Output File=i1r3d3.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.280860	0.000133570	0.000185000
20000.0	0.500340	0.000564300	0.00104000
30000.0	0.620000	0.00113810	0.00228000
40000.0	0.688200	0.00175940	0.00368000
50000.0	0.719200	0.00237500	0.00510000
60000.0	0.737800	0.00298300	0.00650000
70000.0	0.744000	0.00357200	0.00784000
80000.0	0.737800	0.00412300	0.00913000
90000.0	0.731600	0.00463600	0.0104000
100000.	0.719200	0.00514900	0.0116000
110000.	0.496620	0.00552900	0.0126000
120000.	0.316820	0.00568100	0.0131000
130000.	0.211420	0.00571900	0.0133000
140000.	0.145080	0.00571900	0.0133000
150000.	0.102300	0.00566200	0.0133000
160000.	0.0731600	0.00560500	0.0131000
170000.	0.0530720	0.00551000	0.0129000
180000.	0.0388740	0.00539600	0.0126000
190000.	0.0287680	0.00524400	0.0123000
200000.	0.0213900	0.00507300	0.0119000
210000.	0.0159960	0.00486400	0.0114000
220000.	0.0120900	0.00463600	0.0108000
230000.	0.00911400	0.00440800	0.0103000
240000.	0.00694400	0.00418000	0.00973000
250000.	0.00528860	0.00393300	0.00915000
260000.	0.00404860	0.00368600	0.00858000
270000.	0.00310620	0.00343900	0.00802000
280000.	0.00239320	0.00321100	0.00747000
290000.	0.00184140	0.00298300	0.00694000
300000.	0.00142600	0.00277400	0.00644000

Table 4. Concentration history a 500 m for the inventory two (Cm-245, Np-237, and U-233) simulations of problem 8.1.

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
Retardation Set 1 and 0m Dispersivity, Output File=i2r1d1.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.000000	0.000000	0.000000
20000.0	0.000000	0.000000	0.000000
30000.0	0.000000	0.000000	0.000000
40000.0	0.000000	0.000000	0.000000
50000.0	0.000000	0.000000	0.000000
60000.0	0.000000	0.000000	0.000000
70000.0	0.000000	0.000000	0.000000
80000.0	0.000000	0.000000	0.000000
90000.0	0.000000	0.000000	0.000000
100000.	0.000000	0.000000	0.000000
110000.	0.000000	0.000000	0.000000
120000.	0.000000	0.000000	0.000000
130000.	0.000000	0.000000	0.000000
140000.	0.000000	0.000000	0.000000
150000.	0.000000	0.000000	0.000000
160000.	0.000000	0.000000	4.42700e-009
170000.	0.000000	0.000000	2.96400e-008
180000.	0.000000	0.000000	0.116850
190000.	0.000000	0.000000	0.325850
200000.	0.000000	0.000000	0.438900
210000.	0.000000	0.000000	0.501600
220000.	0.000000	0.000000	0.537700
230000.	0.000000	0.000000	0.552900
240000.	0.000000	0.000000	0.557650
250000.	0.000000	0.000000	0.555750
260000.	0.000000	0.000000	0.548150
270000.	0.000000	0.000000	0.548150
280000.	0.000000	8.97000e-011	0.542450
290000.	0.000000	5.96850e-010	0.544350
300000.	0.000000	1.78020e-009	0.547200
Retardation Set 2 and 0m Dispersivity, Output File=i2r2d1.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.000000	0.000000	0.000000
20000.0	0.000000	0.000000	0.000000
30000.0	0.0372000	1.00740e-005	2.78350e-007
40000.0	0.0268000	0.000109710	0.113050
50000.0	0.0119000	0.000196650	0.213750

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
60000.0	0.00527000	0.000283590	0.305900
70000.0	0.00233000	0.000383640	0.398050
80000.0	0.00103000	0.000501630	0.482600
90000.0	0.000457000	0.00986700	0.565250
100000.	0.000202000	0.610650	0.632700
110000.	8.95000e-005	0.890100	0.668800
120000.	3.96000e-005	0.952200	0.685900
130000.	6.71000e-006	0.959100	0.530100
140000.	3.57000e-008	0.959100	0.320150
150000.	2.42000e-010	0.959100	0.261250
160000.	1.69000e-012	0.952200	0.204250
170000.	1.18000e-014	0.952200	0.149150
180000.	8.26000e-017	0.945300	0.0959500
190000.	5.76000e-019	0.931500	0.0494000
200000.	4.01000e-021	0.349830	0.0160550
210000.	2.80000e-023	0.0883200	0.00417050
220000.	1.95000e-025	0.0231150	0.00112100
230000.	1.36000e-027	0.00627900	0.000309700
240000.	0.000000	0.00174570	8.68300e-005
250000.	0.000000	0.000491970	2.46050e-005
260000.	0.000000	0.000139380	6.99200e-006
270000.	0.000000	3.97440e-005	1.99500e-006
280000.	0.000000	1.13160e-005	5.69050e-007
290000.	0.000000	3.22920e-006	1.62450e-007
300000.	0.000000	9.24600e-007	4.63600e-008
Retardation Set 3 and 0m Dispersivity, Output File=i2r3d1.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.000000	0.000000	0.000000
20000.0	0.000000	0.000000	0.0688750
30000.0	0.000000	0.000000	0.176700
40000.0	0.000000	0.621000	0.267900
50000.0	0.000000	0.979800	0.305900
60000.0	0.000000	0.986700	0.340100
70000.0	0.000000	0.986700	0.372400
80000.0	0.000000	0.979800	0.403750
90000.0	0.000000	0.979800	0.432250
100000.	0.000000	0.972900	0.460750
110000.	0.000000	0.972900	0.488300
120000.	0.000000	0.966000	0.119700
130000.	0.000000	0.966000	0.0549100
140000.	0.000000	0.356730	0.00736250
150000.	0.000000	0.0123510	0.000271700

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
160000.	0.000000	0.000507150	1.14950e-005
170000.	0.000000	2.22870e-005	5.14900e-007
180000.	0.000000	1.08330e-006	2.85000e-008
190000.	0.000000	9.10800e-008	3.51500e-009
200000.	0.000000	2.10450e-008	1.01650e-009
215000.	0.000000	4.73340e-009	2.24200e-010
225000.	0.000000	1.85610e-009	8.38850e-011
235000.	0.000000	7.31400e-010	3.11600e-011
245000.	9.21000e-011	2.86350e-010	1.14950e-011
255000.	1.73000e-010	1.12470e-010	4.20850e-012
265000.	1.34000e-010	4.34010e-011	1.52000e-012
275000.	8.10000e-011	1.66980e-011	5.45300e-013
285000.	4.26000e-011	6.32730e-012	1.92850e-013
295000.	2.08000e-011	2.38050e-012	6.71650e-014
305000.	9.73000e-012	8.83200e-013	2.29900e-014
Retardation Set 1and 50m Dispersivity, Output File=i2r1d2.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	1.13000e-026	3.07740e-015	1.28250e-012
20000.0	3.29000e-023	1.33170e-011	5.19650e-009
30000.0	2.52000e-021	1.52490e-009	4.86400e-007
40000.0	4.27000e-020	3.89850e-008	9.69000e-006
50000.0	3.16000e-019	4.37460e-007	8.28400e-005
60000.0	1.38000e-018	2.91870e-006	0.000419900
70000.0	4.21000e-018	1.36620e-005	0.00148200
80000.0	9.82000e-018	4.91280e-005	0.00406600
90000.0	1.87000e-017	0.000144900	0.00920550
100000.	3.03000e-017	0.000367770	0.0179550
110000.	4.31000e-017	0.000821100	0.0313500
120000.	5.50000e-017	0.00165600	0.0499700
130000.	6.42000e-017	0.00308430	0.0741950
140000.	6.94000e-017	0.00534060	0.104500
150000.	7.03000e-017	0.00869400	0.140600
160000.	6.72000e-017	0.0135240	0.180500
170000.	6.10000e-017	0.0200790	0.223250
180000.	5.30000e-017	0.0287730	0.262200
190000.	4.43000e-017	0.0398820	0.296400
200000.	3.57000e-017	0.0536130	0.323950
210000.	2.78000e-017	0.0703800	0.345800
220000.	2.11000e-017	0.0897000	0.362900
230000.	1.55000e-017	0.111090	0.375250
240000.	1.12000e-017	0.134550	0.382850
250000.	7.87000e-018	0.160080	0.387600

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
260000.	5.42000e-018	0.185610	0.389500
270000.	3.66000e-018	0.208380	0.389500
280000.	2.43000e-018	0.228390	0.387600
290000.	1.59000e-018	0.244950	0.383800
300000.	1.02000e-018	0.258750	0.378100
Retardation Set 2 and 50m Dispersivity, Output File=i2r2d2.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.000456000	1.46280e-007	2.39400e-005
20000.0	0.0167000	3.22230e-005	0.00462650
30000.0	0.0308000	0.000685170	0.0364800
40000.0	0.0213000	0.00582360	0.101650
50000.0	0.0110000	0.0255300	0.184300
60000.0	0.00512000	0.0724500	0.269800
70000.0	0.00231000	0.151110	0.351500
80000.0	0.00103000	0.258060	0.426550
90000.0	0.000456000	0.379500	0.494950
100000.	0.000202000	0.498180	0.554800
110000.	8.93000e-005	0.599610	0.606100
120000.	3.45000e-005	0.682410	0.606100
130000.	8.64000e-006	0.752100	0.498750
140000.	1.65000e-006	0.793500	0.387600
150000.	2.85000e-007	0.800400	0.310650
160000.	4.67000e-008	0.779700	0.252700
170000.	7.47000e-009	0.724500	0.204250
180000.	1.18000e-009	0.643770	0.163400
190000.	1.84000e-010	0.542340	0.128250
200000.	2.88000e-011	0.437460	0.0988000
210000.	4.48000e-012	0.345000	0.0757150
220000.	6.96000e-013	0.267720	0.0573800
230000.	1.08000e-013	0.205620	0.0431300
240000.	1.69000e-014	0.155940	0.0322050
250000.	2.63000e-015	0.117300	0.0239400
260000.	4.10000e-016	0.0876300	0.0177650
270000.	6.41000e-017	0.0654810	0.0131100
280000.	1.00000e-017	0.0485760	0.00969000
290000.	1.57000e-018	0.0359490	0.00708700
300000.	2.47000e-019	0.0264960	0.00519650
Retardation Set 3 and 50m Dispersivity, Output File=i2r3d2.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	1.18000e-014	0.000130410	0.00283100
20000.0	2.04000e-011	0.0258750	0.0589950
30000.0	9.37000e-010	0.204930	0.151050

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
40000.0	9.62000e-009	0.507150	0.230850
50000.0	4.35000e-008	0.731400	0.292600
60000.0	1.17000e-007	0.862500	0.339150
70000.0	2.23000e-007	0.924600	0.377150
80000.0	3.26000e-007	0.952200	0.410400
90000.0	3.93000e-007	0.966000	0.441750
100000.	4.08000e-007	0.966000	0.470250
110000.	3.75000e-007	0.966000	0.448400
120000.	3.12000e-007	0.938400	0.206150
130000.	2.40000e-007	0.759000	0.0978500
140000.	1.72000e-007	0.469890	0.0494950
150000.	1.17000e-007	0.251850	0.0245100
160000.	7.54000e-008	0.126270	0.0117800
170000.	4.69000e-008	0.0607890	0.00553850
180000.	2.81000e-008	0.0286350	0.00257450
190000.	1.63000e-008	0.0133170	0.00118750
200000.	9.22000e-009	0.00612030	0.000542450
210000.	5.05000e-009	0.00280140	0.000247950
220000.	2.69000e-009	0.00127650	0.000113050
230000.	1.38000e-009	0.000582360	5.13000e-005
240000.	6.84000e-010	0.000264960	2.32750e-005
250000.	3.29000e-010	0.000120060	1.05450e-005
260000.	1.55000e-010	5.46480e-005	4.81650e-006
270000.	7.12000e-011	2.48400e-005	2.18500e-006
280000.	3.23000e-011	1.13160e-005	9.97500e-007
290000.	1.45000e-011	5.13360e-006	4.53150e-007
300000.	6.42000e-012	2.33910e-006	2.06150e-007
Retardation Set 1 and 500m Dispersivity, Output File=i2r1d3.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	4.05000e-015	6.44460e-006	2.59350e-005
20000.0	4.68000e-012	0.000507150	0.000826500
30000.0	1.49000e-010	0.00320850	0.00395200
40000.0	1.10000e-009	0.00910800	0.0101650
50000.0	3.71000e-009	0.0178710	0.0195700
60000.0	7.72000e-009	0.0290490	0.0318250
70000.0	1.16000e-008	0.0418140	0.0466450
80000.0	1.39000e-008	0.0557520	0.0635550
90000.0	1.41000e-008	0.0703800	0.0823650
100000.	1.25000e-008	0.0855600	0.102600
110000.	1.00000e-008	0.100740	0.123500
120000.	7.45000e-009	0.115230	0.140600
130000.	5.18000e-009	0.128340	0.152000

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
140000.	3.42000e-009	0.137310	0.160550
150000.	2.16000e-009	0.143520	0.165300
160000.	1.32000e-009	0.147660	0.169100
170000.	7.75000e-010	0.149040	0.171000
180000.	4.44000e-010	0.149730	0.171950
190000.	2.48000e-010	0.148350	0.171950
200000.	1.35000e-010	0.146970	0.171950
210000.	7.23000e-011	0.144900	0.171000
220000.	3.80000e-011	0.142140	0.170050
230000.	1.96000e-011	0.139380	0.168150
240000.	9.98000e-012	0.136620	0.167200
250000.	5.02000e-012	0.133170	0.165300
260000.	2.49000e-012	0.130410	0.163400
270000.	1.23000e-012	0.126960	0.160550
280000.	5.97000e-013	0.123510	0.158650
290000.	2.88000e-013	0.120750	0.155800
300000.	1.38000e-013	0.117300	0.153900
Retardation Set 2and 500m Dispersivity, Output File=i2r2d3.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	0.0353000	0.00586500	0.00441750
20000.0	0.0396000	0.0425730	0.0248900
30000.0	0.0258000	0.0952200	0.0574750
40000.0	0.0142000	0.151110	0.0969000
50000.0	0.00726000	0.204240	0.141550
60000.0	0.00355000	0.253920	0.187150
70000.0	0.00169000	0.300150	0.233700
80000.0	0.000793000	0.342240	0.281200
90000.0	0.000367000	0.380190	0.326800
100000.	0.000168000	0.415380	0.372400
110000.	6.63000e-005	0.441600	0.373350
120000.	2.32000e-005	0.435390	0.340100
130000.	8.19000e-006	0.410550	0.311600
140000.	2.93000e-006	0.380880	0.286900
150000.	1.06000e-006	0.351900	0.266000
160000.	3.88000e-007	0.323610	0.247000
170000.	1.43000e-007	0.298770	0.230850
180000.	5.31000e-008	0.275310	0.215650
190000.	1.98000e-008	0.254610	0.201400
200000.	7.45000e-009	0.235290	0.189050
210000.	2.81000e-009	0.218040	0.177650
220000.	1.06000e-009	0.202170	0.167200
230000.	4.05000e-010	0.187680	0.157700

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
240000.	1.54000e-010	0.175260	0.149150
250000.	5.91000e-011	0.162840	0.140600
260000.	2.26000e-011	0.152490	0.132050
270000.	8.71000e-012	0.142140	0.125400
280000.	3.35000e-012	0.133170	0.118750
290000.	1.29000e-012	0.124200	0.112100
300000.	5.01000e-013	0.116610	0.105450
Retardation Set 3 and 500m Dispersivity, Output File=i2r3d3.GV			
1.00000e-006	0.000000	0.000000	0.000000
10000.0	8.54000e-006	0.0683100	0.0135850
20000.0	0.000187000	0.206310	0.0515850
30000.0	0.000417000	0.326370	0.0997500
40000.0	0.000459000	0.422970	0.150100
50000.0	0.000368000	0.501630	0.201400
60000.0	0.000250000	0.565800	0.250800
70000.0	0.000153000	0.618930	0.299250
80000.0	8.72000e-005	0.662400	0.343900
90000.0	4.75000e-005	0.696900	0.387600
100000.	2.50000e-005	0.731400	0.427500
110000.	1.28000e-005	0.688620	0.354350
120000.	6.41000e-006	0.577530	0.278350
130000.	3.08000e-006	0.480240	0.228000
140000.	1.43000e-006	0.402270	0.190950
150000.	6.49000e-007	0.339480	0.162450
160000.	2.90000e-007	0.289110	0.139650
170000.	1.28000e-007	0.247710	0.121600
180000.	5.60000e-008	0.213210	0.105450
190000.	2.44000e-008	0.184230	0.0929100
200000.	1.06000e-008	0.160770	0.0819850
210000.	4.58000e-009	0.140070	0.0724850
220000.	1.98000e-009	0.122820	0.0643150
230000.	8.53000e-010	0.107640	0.0571900
240000.	3.68000e-010	0.0952200	0.0510150
250000.	1.58000e-010	0.0841800	0.0455050
260000.	6.81000e-011	0.0745200	0.0407550
270000.	2.93000e-011	0.0660330	0.0364800
280000.	1.26000e-011	0.0587190	0.0327750
290000.	5.43000e-012	0.0523020	0.0294500
300000.	2.33000e-012	0.0466440	0.0265050

3 PROBLEM 8.2: TWO-DIMENSIONAL TRANSPORT BETWEEN INJECTION AND PRODUCTION WELLS

3.1 Problem Description and Objectives

This problem simulates an injection and production well in a homogeneous aquifer with a line source placed between the wells. The wells are assumed to be fully penetrating and the flow is two-dimensional. The source is a three chain radionuclide ‘band release’, which includes decay and ingrowth occurring within the source. The wells are 1,020 m apart and the source is 10 m long placed 10 m away from the injection well perpendicular to a line connecting the two wells. Dispersion occurs in the longitudinal and transverse directions. The aquifer is 100m thick and the porosity is 0.01. The production/injection rate is 1088.9 m^3/year. The problem uses decay chain 1 and retardation set 2 presented in Section 2. The test assumptions include:

- The aquifer is uniform and isotropic.
- The background velocity is zero.
- The flow between the wells is at steady-state.
- The domain is infinite.
- Sorption is in equilibrium.

The objective of this benchmark test is to verify a the transport code in a two dimensional flow field with solute decay and ingrowth. The required output is the concentration through time at the y-axis (mid point between wells) and the concentration vs. distance along the y-axis at peak total radionuclide flux across the axis.

3.2 TETRAD Simulation

The simulation approach used with the TETRAD simulator for problem 8.2 was similar to the approach used in problem 8.1. The simulation was performed in three separate runs: (1) run the flow field to steady-state with injection/production rate, (2) run the transport simulation during the source release period with initial pressure from the run 1, and (3) run the transport simulation with the source turned off with initial pressure and nuclide concentration from run 2. During the source release run, the grid block volume within the source area was increased by a factor of 1.e+11 to maintain a non-depleting source (i.e., source concentrations change due to decay and ingrowth, but not due to advection out of the source area). The ‘BVMULT’ keyword was not used in run 3 and the source area was allowed to deplete over time. The 2-D source could not be turned off mid-simulation as was done in problem 8.1, because the former source grid blocks must continue to participate in the continuing simulation.

The simulation grid used quarter symmetry and the grid block size was allowed to increase with distance away from the injection well and source. The simulation only included the injection well and used a constant head boundary at the center between wells. The constant head boundary have resulted in some differences with the analytic solution because solute movement out of the domain in purely advective when using the ‘AQUIFER’ keywords (i.e., dispersive transport through the boundaries was neglected). The production rate was reduced by a factor of two. The liquid viscosity was calculated internally within the TETRAD simulator using the Gottfried temperature relationship. Table 5 summarizes the TETRAD simulation parameters.

The boundary conditions away from the constant head divide between wells used a TETRAD specific approximation to an infinite aquifer. The TETRAD semi-analytic aquifer boundary condition was implemented using the “AQUIFER” and SAINFLIN” keywords. This boundary condition allows pressure behavior at the model boundary to mimics an infinite aquifer within a finite domain. The ‘SAINFLIN’ keyword pressure boundary probably provided a good approximation for flow in a limited simulation domain.

Table 6 provides the cumulative contaminant flux across the center line between the two wells and Table 7 provides the contaminant concentrations versus distance along the axis at 100,000 years. Figure 3 illustrates the steady-state aquifer pressure head resulting from the injection and production well operation. Figure 4 illustrates the each contaminant concentration versus distance along the y-axis at 100,000 years.

Table 5. TETRAD simulation parameters for problem 8.2.

Parameter	Value
Porosity	0.01
Perrmeability (mD)	10.
Liquid Density (Kg/m^3)	1000
Viscosity (mPa S)	1.17
Temperature (degree C)	15.
Particle Density (Kg/m^3)	2650.
Longitudinal Dispersivity (m)	50.
Transverse Dispersivity (m)	5.

Table 6. Contaminant cumulative flux across the center line between wells for problem 8.2.

Time (yr)	U-234 (Ci)	Th-230 (Ci)	Ra-226 (Ci)
0.000e+000	0.000e+000	0.000e+000	0.000e+000
1.000e+003	9.753e-006	1.359e-009	1.497e-003
5.000e+003	4.339e+001	2.869e-002	9.093e+001
1.000e+004	5.654e+003	9.148e+000	3.177e+003
1.500e+004	4.942e+004	1.402e+002	1.962e+004
2.000e+004	1.732e+005	7.368e+002	6.504e+004
2.500e+004	3.969e+005	2.309e+003	1.565e+005
3.000e+004	7.198e+005	5.392e+003	3.098e+005
3.500e+004	1.131e+006	1.046e+004	5.384e+005
4.000e+004	1.616e+006	1.788e+004	8.532e+005
4.500e+004	2.163e+006	2.793e+004	1.263e+006
5.000e+004	2.758e+006	4.081e+004	1.773e+006
5.500e+004	3.393e+006	5.668e+004	2.389e+006
6.000e+004	4.058e+006	7.558e+004	3.114e+006
6.500e+004	4.749e+006	9.756e+004	3.950e+006
7.000e+004	5.458e+006	1.226e+005	4.899e+006
7.500e+004	6.182e+006	1.508e+005	5.962e+006
8.000e+004	6.919e+006	1.821e+005	7.139e+006
8.500e+004	7.663e+006	2.164e+005	8.430e+006
9.000e+004	8.413e+006	2.538e+005	9.834e+006
9.500e+004	9.170e+006	2.941e+005	1.135e+007
1.000e+005	9.926e+006	3.376e+005	1.298e+007
1.050e+005	1.068e+007	3.839e+005	1.472e+007

Time (yr)	U-234 (Ci)	Th-230 (Ci)	Ra-226 (Ci)
1.100e+005	1.144e+007	4.331e+005	1.655e+007
1.150e+005	1.217e+007	4.851e+005	1.845e+007
1.200e+005	1.284e+007	5.396e+005	2.040e+007
1.250e+005	1.344e+007	5.964e+005	2.239e+007
1.300e+005	1.396e+007	6.547e+005	2.439e+007
1.350e+005	1.441e+007	7.144e+005	2.640e+007
1.400e+005	1.479e+007	7.748e+005	2.841e+007
1.450e+005	1.513e+007	8.362e+005	3.041e+007
1.500e+005	1.542e+007	8.977e+005	3.238e+007
1.550e+005	1.568e+007	9.595e+005	3.432e+007
1.600e+005	1.591e+007	1.021e+006	3.623e+007
1.650e+005	1.611e+007	1.083e+006	3.810e+007
1.700e+005	1.630e+007	1.144e+006	3.993e+007
1.750e+005	1.646e+007	1.205e+006	4.171e+007
1.800e+005	1.661e+007	1.265e+006	4.344e+007
1.850e+005	1.675e+007	1.324e+006	4.512e+007
1.900e+005	1.688e+007	1.382e+006	4.674e+007
1.950e+005	1.699e+007	1.438e+006	4.832e+007
2.000e+005	1.709e+007	1.494e+006	4.983e+007

Table 7. Contaminant concentration along the y-axis after 100,000 years for problem 8.2.

Distance (m)	U-234 (Ci/m^3)	Th-230 (Ci/m^3)	Ra-226 (Ci/m^3)
0.500000	0.651000	0.0495900	2.04000
2.00000	0.651000	0.0495900	2.04000
4.00000	0.651000	0.0495900	2.04000
7.00000	0.651000	0.0495900	2.04000
12.0000	0.651000	0.0494000	2.04000
19.0000	0.651000	0.0492100	2.03000
29.0000	0.644800	0.0488300	2.01000
44.0000	0.638600	0.0478800	1.96000
65.0000	0.626200	0.0457900	1.87000
95.0000	0.598300	0.0425600	1.71000
137.000	0.559860	0.0376200	1.47000
197.000	0.507780	0.0311600	1.15000
281.000	0.447020	0.0243200	0.824000
395.000	0.364560	0.0160930	0.513000
545.000	0.225060	0.00742900	0.236000
731.000	0.0731600	0.00178980	0.0595000
953.000	0.00985800	0.000188670	0.00672000
1193.00	0.000620000	9.76600e-006	0.000375000
1433.00	2.07080e-005	2.79300e-007	1.16000e-005

Distance (m)	U-234 (Ci/m^3)	Th-230 (Ci/m^3)	Ra-226 (Ci/m^3)
1673.00	3.95560e-007	4.67400e-009	2.10000e-007
1913.00	4.48880e-009	4.76900e-011	2.32000e-009
2153.00	2.98840e-011	2.86900e-013	1.53000e-011
2393.00	1.02300e-013	9.04400e-016	5.27000e-014

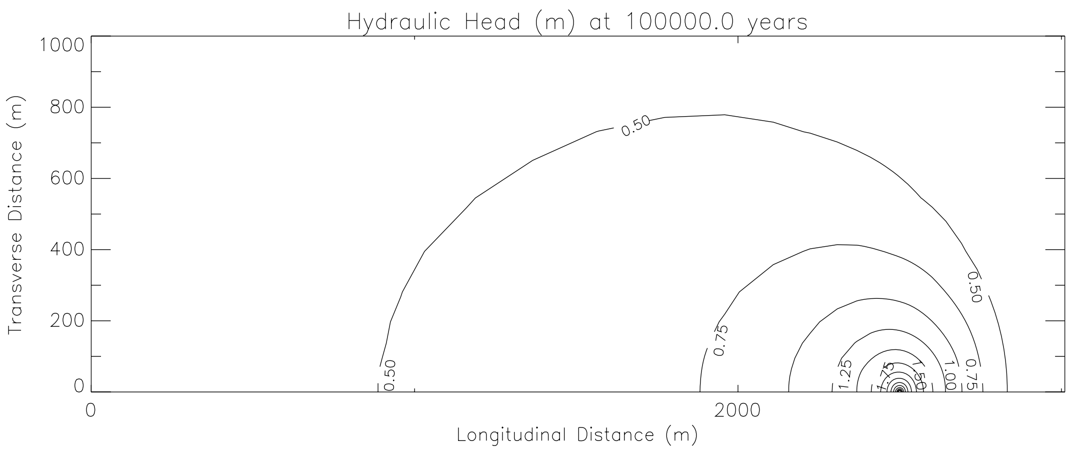

Figure 3. Aquifer pressure head for problem 8.2.

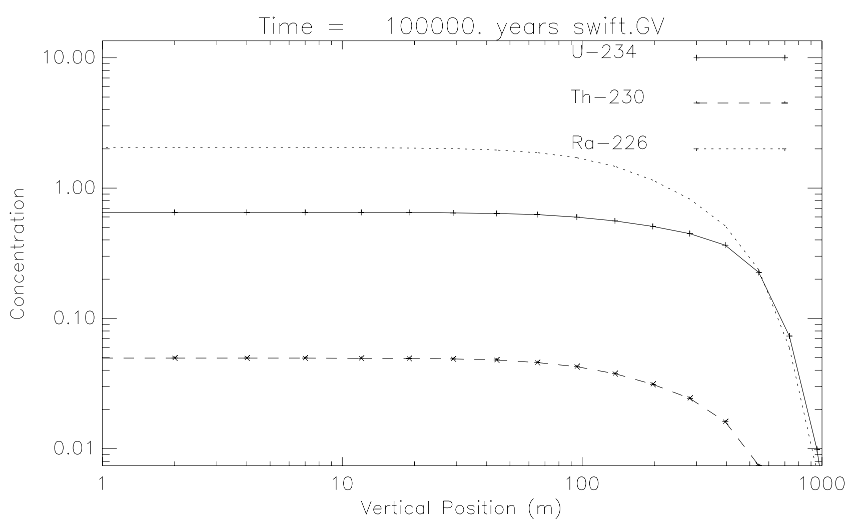

Figure 4. Contaminant concentration (Ci/m^3) along the y-axis after 100,000 years for problem 8.2.

4 PROBLEM EPA 2D: TWO-DIMENSIONAL TRANSPORT FROM LIGHT INJECTATE IN A DIPPING AQUIFER

4.1 Problem Description and Objectives

This problem simulates injectate movement from a fully penetrating injection well completed in an infinite aquifer. The injectate is less dense than the reservoir fluid. The reservoir dip is 0.5 degrees down dip of the well to 5,000 ft up dip. The dip increases to 0.75 degrees from 5,000 ft up dip to 15,000 ft up dip and increases again to 1.0 degree beyond 15,000 ft up dip. The problem considers advective and dispersive flow only. Molecular diffusion is neglected. The test assumptions include:

- The aquifer has a uniform thickness and is isotropic.
- The background velocity is zero.
- The domain is infinite.
- Flow is transient
- Molecular diffusion is negligible.

The objective of this problem is the assess the code's ability to simulate density driven flow with hydrodynamic dispersion. The required output is the normalized 1.e-6 and 1.e-12 isopleths at 1, 5, 100, and 10,000 years.

4.2 TETRAD Simulation

This simulation was accomplished by defining the dipping formation surface elevation at each simulation cell with the TETRAD 'FTOPS' keyword.The simulation initial conditions are hydrostatic pressure. The reservoir and injectate properties are provided in Table 8.

The density effects of a light injectate and dipping aquifer are easily simulated with TETRAD's multiphase/multicomponent capabilities. The required output is concentration isopleths 1.e-6 and 1.e-12. Density effects at these concentrations are negligible. Concentration isopleths values in the 1 to 0.10 range provide a better indication of the plume under density driven flow conditions.

The simulation domain was approximately 9,000 m x 3,000 m and used 720 x 240 grid blocks. The grid block size was a uniform 12.7 m in the horizontal directions. This was the model grid used in the "y10k2d" input file provided by GeoTrans, Inc. Figure 5 illustrates the 2-D simulation grid. The boundary conditions were parameterized using the TETRAD specific approximation to an infinite aquifer. The TETRAD semi-analytic aquifer boundary condition was implemented using the "AQUIFER" and SAINFLIN" keywords. This boundary condition allows transient pressure behavior at the model boundary, which mimics an infinite aquifer within a finite domain. This is accomplished using an semi-analytical transient solution for aquifer pressure change coded within the TETRAD simulator. No numerical problems were encountered with the simulation and the relative mass balance error was 1e-5 after 10,000 years. The simulation results show a mostly circular plume during the injection well operation, which slowly advects and disperses up dip because the injectate is less dense than the reservoir. Figure 6 illustrates the plume after 1, 5, 100, and 10,000 years. The 1e-6 and 1e-12 isopleths are illustrated in red, while the 0.2, 0.4, 0.6, and 8. isopleths are illustrated in black.

Table 8. TETRAD simulation parameters for problem EPA 2D.

Parameter	Value
Porosity	0.30
Perrmeability (mD)	750.

Parameter	Value
Reservoir Density (Kg/m^3)	1059.34
Reservoir Thickness (m)	12.2
Injectate Density (Kg/m^3)	999.38
Reservoir Viscosity (mPa S)	0.583
Injectate Viscosity (mPa S)	0.413
Temperature (degree C)	155.
Reference Temperature for Fluids (degrees C)	155.
Reference Pressure for Fluids (Kpa)	16031.
Particle Density (Kg/m^3)	2650.
Water Compressibility (1/KPa)	4.351e-6
Rock Compressibility (1/KPa)	3.0e-6
Longitudinal Dispersivity (m)	30.48
Transverse Dispersivity (m)	4.572
Molecular Diffusivity (m^2/day)	0.
Injection Rate (m^3/day) for 8 years	2725.2
Well Radius (m)	0.1015

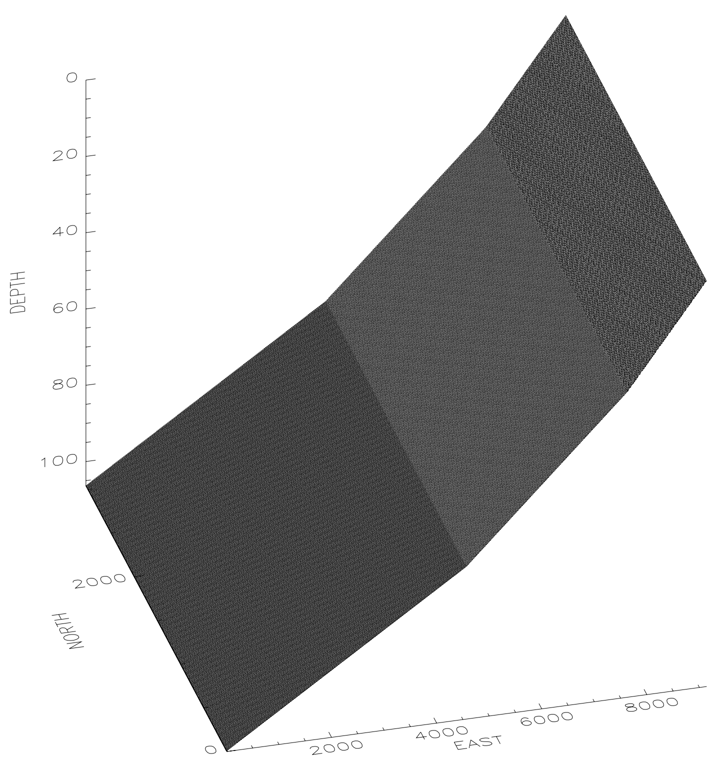

Figure 5. Problem EPA 2D simulation grid.

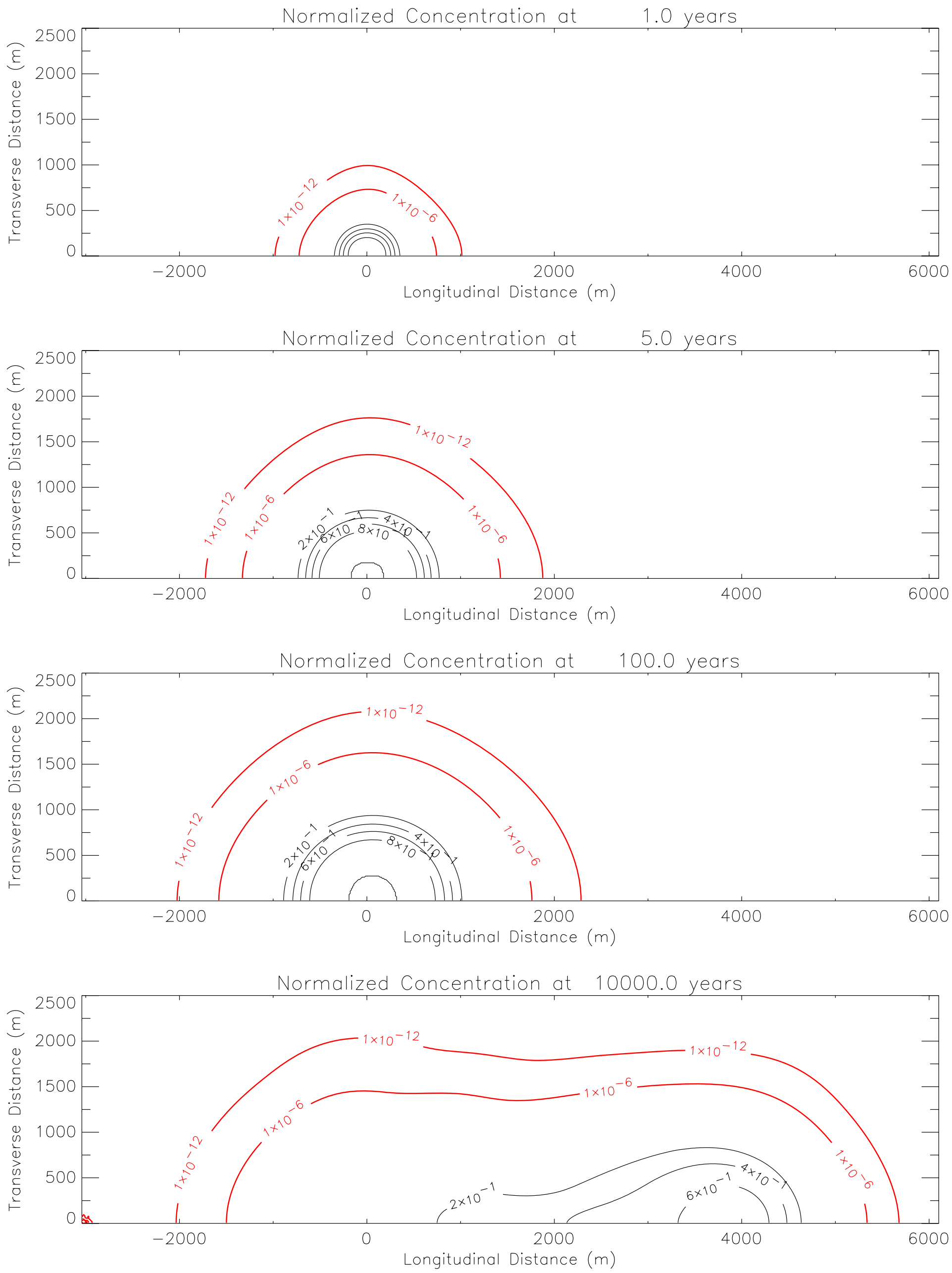

Figure 6. Problem EPA 2D plume concentration after 1, 5, 100 and 10,000 years.

5 PROBLEM EPA 2F: TWO-DIMENSIONAL TRANSPORT FROM LIGHT INJECTATE IN A DIPPING AQUIFER WITH A BACKGROUND VELOCITY

5.1 Problem Description and Objectives

This problem is similar to problem EPA 2D and simulates injectate movement from a fully penetrating injection well completed in an infinite aquifer. However, the problem includes a 0.5 ft/yr downdip background velocity. The injectate is less dense than the reservoir fluid. The reservoir dip is uniform and 1.5 degrees across the aquifer. The problem considers advective and dispersive flow and molecular diffusion.The test assumptions include:

- The aquifer has a uniform thickness, uniform dip and is isotropic.
- The background velocity is 0.5 ft/yr down dip.
- The domain is infinite.
- Flow is transient

The objective of this problem is the assess the code's ability to simulate density driven flow with dispersion and diffusion in a flowing aquifer. The required output is the normalized 1.e-6 and 1.e-12 isopleths at 1, 5, 100, and 10,000 years.

5.2 TETRAD Simulation

This simulation is a difficult problem because of the aquifer is assumed to be infinite, the injection rate is large (500 gpm), injection period is long (8 years), and a uniform background velocity must be maintained. The semi-analytic aquifer boundary condition ('SAINFLIN' keyword) used in problem EPA 2D could not be used for this problem because the semi-analytical boundary conditions would eventually equilibrate to hydrostatic and a background velocity must be maintained. However, the density effects of a heavy injectate and dipping aquifer are easily simulated by TETRAD's multiphase/multicomponent capabilities. Also, the dipping aquifer along with the specified pore space and liquid compressibility will not maintain a uniform velocity down dip with the specified problem parameters. As hydrostatic pressure increases down dip, the pore space and liquid density changes resulting in a slightly non-uniform velocity field.

This simulation was parameterized similar to problem EPA 2D and was accomplished by defining the dipping formation surface elevation at each simulation cell with the TETRAD 'FTOPS' keyword. The background velocity was parameterized by specifying constant pressure boundary conditions updip and downdip of the injection well. The 'AQUIFER' and 'SSTATE' keywords were used to set up and down gradient Dirichlet boundary conditions and establish the pressure gradient needed for a 0.5 ft/yr linear velocity. Table 9 provides the TETRAD parameters used in this simulation.

The simulation domain was approximately 15,000 m x 5,000 m and used 720 x 240 grid blocks. The grid block size was a uniform 20.32 m in the horizontal directions. This was the model grid used in the "y10k2f" input file provided by GeoTrans, Inc. Figure 7 illustrates the 2-D simulation grid. No numerical problems were encountered with the simulation and the relative injectate mass balance was 1e-3 after 10,000 years. A slight increase in model pressure was seen near the model boundaries indicating the model only approximated an infinite aquifer and the TETRAD numerical solution may be slightly different than an analytical or semi-analytical type solution.

The simulation results show a mostly circular plume during the injection well operation, which is subject to down dip movement due to the background velocity and up dip movement due to the injectate's buoyancy in the reservoir. The updip velocity due to injectate buoyancy overtakes the down dip velocity and the plume mostly migrates updip. Although, the area of the plume at very low concentrations moves down dip because the density difference between the plume and the reservoir is negligible. The causes a sharper up dip plume front than the down dip plume tail. Figure 8 illustrates the plume at the end of 1, 5, 100, and 10,000 years.

Table 9. TETRAD simulation parameters for problem EPA 2F.

Parameter	Value
Porosity	0.30
Permeability (mD)	750.
Reservoir Density (Kg/m^3)	1059.34
Reservoir Thickness (m)	12.2
Injectate Density (Kg/m^3)	999.38
Reservoir Viscosity (mPa S)	0.583
Injectate Viscosity (mPa S)	0.413
Temperature (degree C)	155.
Reference Temperature for Fluids (degrees C)	155.
Reference Pressure for Fluids (KPa)	16031.
Particle Density (Kg/m^3)	2650.
Water Compressibility (1/KPa)	3.0e-6
Rock Compressibility (1/KPa)	3.0e-6
Longitudinal Dispersivity (m)	30.48
Transverse Dispersivity (m)	4.572
Molecular Diffusivity (m^2/day)	4.0e-4
Injection Rate (m^3/day) for 8 years	2725.2
Well Radius (m)	0.1015

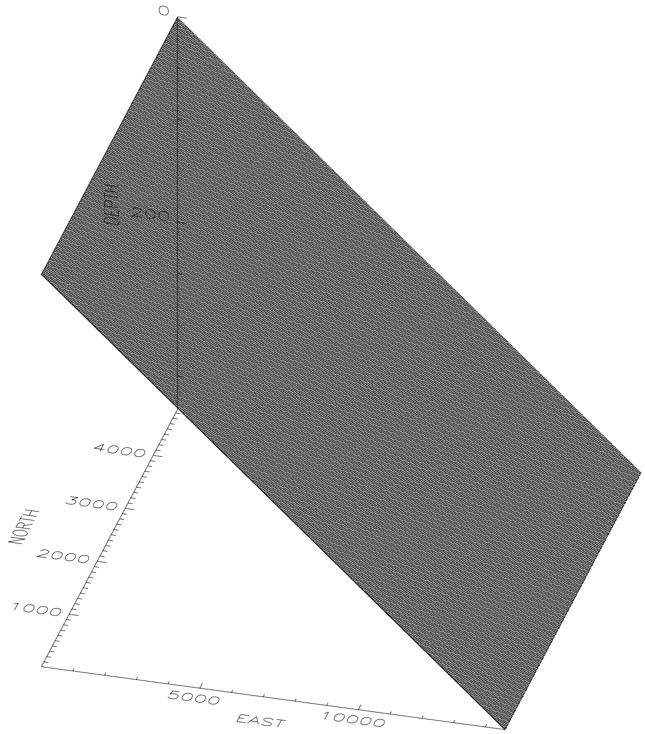

Figure 7. Problem EPA 2F simulation grid.

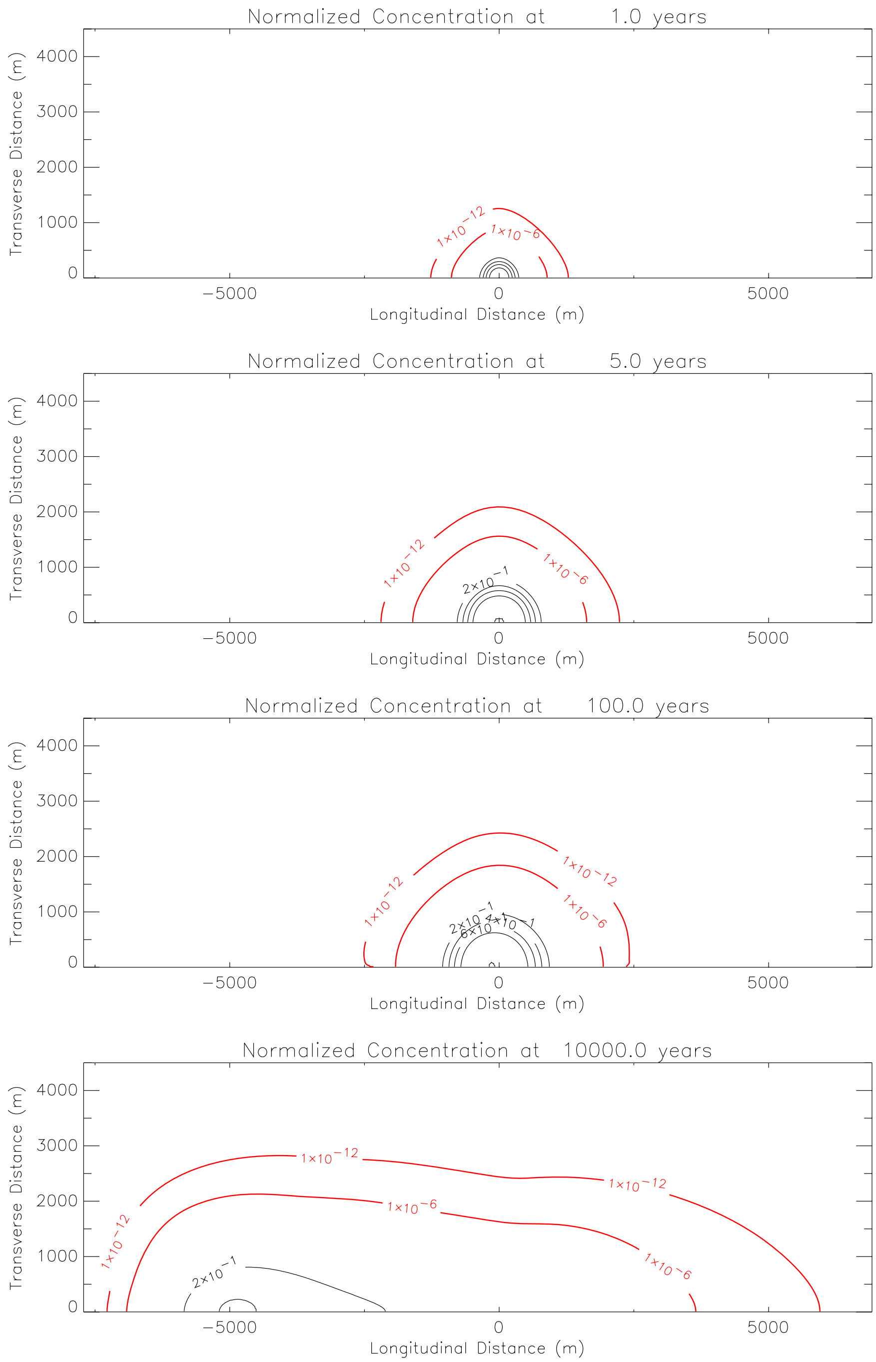

Figure 8. Problem EPA 2F plume concentration after 1, 5, 100 and 10,000 years.

6 PROBLEM 9.1: ONE-DIMENSIONAL TRANSPORT WITH RADIONUCLIDE CHAIN DECAY IN SATURATED FRACTURED POROUS MEDIA

6.1 Problem Description and Objectives

This problem simulates one-dimensional transport from a river channel containing a three chain radionuclide source. The aquifer is assumed to be a fractured porous media with a high fracture permeability and zero matrix permeability. The aquifer is assumed to infinite with a constant fracture velocity. The source undergoes decay as a three chain decay series. The problem uses decay chain 2 and retardation set 3 presented in Section 2. The test assumptions include:

• Flow and transport is one-dimensional.

• Fracture velocity is constant at 500 m/year.

• The domain in semi-infinite.

• Sorption is in equilibrium and only occurs in the matrix media.

• Matrix retardation (R_d), sorption coefficient (K_d), and bulk density (ρ_b) are related via R_d=K_d*ρ_b.

• Fractures are planar and parallel to the flow direction.

• The matrix media has a zero permeability and transport into the media is purely diffusional.

The objective of this problem is to test the simulation code's ability to simulate a fractured rock aquifer. The required output is the concentration through time at a location 500 m down gradient of the source.

6.2 TETRAD Simulation

The simulation approach used to define the decay chain and velocity field is identical to the approach used in problem 8.1. Half symmetry through 1 fracture and matrix block was used to reduce the computational burden. Half symmetry placed a zero flux boundary at the fracture midpoint and the matrix midpoint. The simulated half fracture used single grid block of 5.e-5 m in the y-direction and the matrix used 16 grid blocks in the y-direction. The matrix grid block size was increased towards the midpoint at 2.5 m into the matrix.

This problem was parameterized using a single porosity/permeability porous media with different material types for the fracture and matrix. The TETRAD simulator allows simulation of dual porosity/permeability fractured porous media the 'DUAL' keyword, but the matrix grid block discretization is equivalent to the fracture material and a concentration gradient with the matrix block can not be simulated. The fracture was approximated by using large porosity (0.999) to approximate an open flow channel. In this problem, transport into and through the matrix media is purely diffusional. This was approximated by setting the fracture permeability to 1.e-10 mD. The TETRAD parameters are presented in Table 10.

The harmonic average used by TETRAD for calculating inter-grid block transmissibility may result in a slightly different solution than the analytical solution. No numerical problems were encountered and the tracer mass balance was very good with a relative error of 1e-9 magnitude. Figure 9 illustrates the fracture breakthrough at 500 m down gradient. Figure 10 illustrates the matrix breakthrough at 500 m down gradient and approximately 2 cm into the fracture. The fracture concentration history is provided in Table 11 and the matrix concentration history is provided in Table 12.

Table 10. TETRAD simulation parameters for problem 9.1.

Parameter	Value
Half Fracture Width (m)	1.e-4
Fracture Spacing (m)	5
Fracture Porosity	0.999
Fracture Permeability (mD)	192484.
Fracture Tortuosity	1.
Matrix Porosity	5.e-3
Matrix Permeability (mD)	1.0e-10
Fluid Density (Kg/m^3)	1000.
Particle Density (Kg/m^3)	2650.
Temperature (degree C)	15.
Particle Density (Kg/m^3)	2650.
Longitudinal Dispersivity (m)	50.
Molecular Diffusivity (m^2/day)	1.728e-5
Matrix Tortuosity	200.

Table 11. Fracture concentration history at 500 m for problem 9.1.

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
0.0	0.000000	0.000000	0.000000
100.000	2.70000e-028	6.96900e-020	7.55250e-019
1000.00	2.44000e-019	5.97540e-013	7.52400e-013
5000.00	2.03000e-014	1.67670e-009	9.78500e-010
10000.0	9.75000e-013	2.24940e-008	1.20650e-008
15000.0	6.04000e-012	7.93500e-008	4.30350e-008
20000.0	1.73000e-011	1.73880e-007	9.59500e-008
25000.0	3.31000e-011	2.98080e-007	1.71000e-007
30000.0	4.99000e-011	4.45050e-007	2.62200e-007
35000.0	6.41000e-011	6.06510e-007	3.69550e-007
40000.0	7.38000e-011	7.79700e-007	4.87350e-007
45000.0	7.81000e-011	9.52200e-007	6.13700e-007
50000.0	7.76000e-011	1.12470e-006	7.46700e-007
55000.0	7.34000e-011	1.29720e-006	8.84450e-007
60000.0	6.67000e-011	1.46970e-006	1.02600e-006
65000.0	5.86000e-011	1.63530e-006	1.16850e-006
70000.0	5.01000e-011	1.79400e-006	1.31100e-006
75000.0	4.18000e-011	1.94580e-006	1.45350e-006
80000.0	3.43000e-011	2.09760e-006	1.60550e-006
85000.0	2.76000e-011	2.23560e-006	1.74800e-006
90000.0	2.19000e-011	2.37360e-006	1.89050e-006

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
95000.0	1.72000e-011	2.49780e-006	2.03300e-006
100000.	1.33000e-011	2.62200e-006	2.17550e-006
100000.	1.33000e-011	2.62200e-006	2.17550e-006
100001.	1.33000e-011	2.62200e-006	2.17550e-006
100010.	1.33000e-011	2.62200e-006	2.17550e-006
100100.	1.32000e-011	2.62200e-006	2.17550e-006
100200.	1.31000e-011	2.62890e-006	2.17550e-006
100400.	1.30000e-011	2.62890e-006	2.18500e-006
100500.	1.29000e-011	2.63580e-006	2.18500e-006
101000.	1.26000e-011	2.64270e-006	2.20400e-006
105000.	1.02000e-011	2.73240e-006	2.29900e-006
110000.	7.72000e-012	2.82900e-006	2.32750e-006
115000.	5.81000e-012	2.87730e-006	2.29900e-006
120000.	4.34000e-012	2.89110e-006	2.24200e-006
125000.	3.21000e-012	2.87730e-006	2.17550e-006
130000.	2.36000e-012	2.82900e-006	2.09950e-006
135000.	1.73000e-012	2.76690e-006	2.02350e-006
140000.	1.25000e-012	2.69100e-006	1.95700e-006
145000.	9.03000e-013	2.60820e-006	1.89050e-006
150000.	6.48000e-013	2.51850e-006	1.83350e-006
155000.	4.62000e-013	2.42880e-006	1.77650e-006
160000.	3.28000e-013	2.33220e-006	1.71950e-006
165000.	2.32000e-013	2.24250e-006	1.67200e-006
170000.	1.64000e-013	2.15280e-006	1.62450e-006
175000.	1.15000e-013	2.07000e-006	1.57700e-006
180000.	8.02000e-014	1.98030e-006	1.53900e-006
185000.	5.58000e-014	1.90440e-006	1.49150e-006
190000.	3.88000e-014	1.82850e-006	1.45350e-006
195000.	2.69000e-014	1.75260e-006	1.42500e-006
200000.	1.85000e-014	1.68360e-006	1.38700e-006
205000.	1.28000e-014	1.61460e-006	1.35850e-006
210000.	8.78000e-015	1.55250e-006	1.32050e-006
215000.	6.02000e-015	1.49730e-006	1.29200e-006
220000.	4.12000e-015	1.44210e-006	1.26350e-006
225000.	2.82000e-015	1.38690e-006	1.24450e-006
230000.	1.92000e-015	1.33860e-006	1.21600e-006
235000.	1.31000e-015	1.29030e-006	1.18750e-006
240000.	8.89000e-016	1.24200e-006	1.16850e-006
245000.	6.04000e-016	1.20060e-006	1.14000e-006
250000.	4.09000e-016	1.15920e-006	1.12100e-006
255000.	2.77000e-016	1.11780e-006	1.10200e-006
260000.	1.88000e-016	1.08330e-006	1.08300e-006

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
265000.	1.27000e-016	1.04880e-006	1.05450e-006
270000.	8.55000e-017	1.01430e-006	1.03550e-006
275000.	5.77000e-017	9.86700e-007	1.02600e-006
280000.	3.89000e-017	9.52200e-007	1.00700e-006
285000.	2.62000e-017	9.24600e-007	9.88000e-007
290000.	1.76000e-017	8.97000e-007	9.69000e-007
295000.	1.18000e-017	8.76300e-007	9.50000e-007
300000.	7.94000e-018	8.48700e-007	9.38600e-007
305000.	5.33000e-018	8.28000e-007	9.23400e-007

Table 12. Matrix concentration history at 500 m for problem 9.1.

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
0.0	0.000000	0.000000	0.000000
100.000	3.05000e-010	6.70680e-008	1.69100e-009
1000.00	7.76000e-008	1.74570e-006	3.23000e-008
5000.00	5.95000e-007	4.88520e-006	1.95700e-007
10000.0	7.48000e-007	6.17550e-006	4.07550e-007
15000.0	6.61000e-007	6.81720e-006	6.18450e-007
20000.0	5.20000e-007	7.17600e-006	8.24600e-007
25000.0	3.88000e-007	7.45200e-006	1.02600e-006
30000.0	2.81000e-007	7.65900e-006	1.22550e-006
35000.0	1.99000e-007	7.79700e-006	1.41550e-006
40000.0	1.39000e-007	7.93500e-006	1.60550e-006
45000.0	9.66000e-008	8.07300e-006	1.79550e-006
50000.0	6.66000e-008	8.14200e-006	1.97600e-006
55000.0	4.57000e-008	8.21100e-006	2.15650e-006
60000.0	3.12000e-008	8.28000e-006	2.32750e-006
65000.0	2.12000e-008	8.28000e-006	2.49850e-006
70000.0	1.44000e-008	8.34900e-006	2.66000e-006
75000.0	9.77000e-009	8.34900e-006	2.82150e-006
80000.0	6.61000e-009	8.41800e-006	2.98300e-006
85000.0	4.46000e-009	8.41800e-006	3.13500e-006
90000.0	3.01000e-009	8.48700e-006	3.28700e-006
95000.0	2.03000e-009	8.48700e-006	3.42950e-006
100000.	1.36000e-009	8.48700e-006	3.58150e-006
100000.	1.36000e-009	8.48700e-006	3.58150e-006
100001.	1.36000e-009	8.48700e-006	3.58150e-006
100010.	1.36000e-009	8.48700e-006	3.58150e-006
100100.	1.35000e-009	8.41800e-006	3.47700e-006
100200.	1.34000e-009	8.34900e-006	3.31550e-006
100400.	1.32000e-009	8.00400e-006	3.01150e-006

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
100500.	1.31000e-009	7.79700e-006	2.88800e-006
101000.	1.24000e-009	7.03800e-006	2.43200e-006
105000.	7.64000e-010	4.01580e-006	1.33000e-006
110000.	4.19000e-010	2.73930e-006	9.69000e-007
115000.	2.36000e-010	2.10450e-006	7.96100e-007
120000.	1.36000e-010	1.71120e-006	6.90650e-007
125000.	7.99000e-011	1.44900e-006	6.17500e-007
130000.	4.74000e-011	1.24890e-006	5.62400e-007
135000.	2.85000e-011	1.09710e-006	5.18700e-007
140000.	1.72000e-011	9.72900e-007	4.83550e-007
145000.	1.05000e-011	8.76300e-007	4.53150e-007
150000.	6.45000e-012	7.93500e-007	4.27500e-007
155000.	3.97000e-012	7.24500e-007	4.05650e-007
160000.	2.46000e-012	6.65850e-007	3.85700e-007
165000.	1.53000e-012	6.15480e-007	3.68600e-007
170000.	9.51000e-013	5.71320e-007	3.52450e-007
175000.	5.94000e-013	5.32680e-007	3.38200e-007
180000.	3.72000e-013	4.98870e-007	3.24900e-007
185000.	2.34000e-013	4.68510e-007	3.13500e-007
190000.	1.47000e-013	4.40910e-007	3.02100e-007
195000.	9.29000e-014	4.16070e-007	2.92600e-007
200000.	5.87000e-014	3.93990e-007	2.83100e-007
205000.	3.72000e-014	3.73290e-007	2.73600e-007
210000.	2.36000e-014	3.54660e-007	2.66000e-007
215000.	1.50000e-014	3.36720e-007	2.58400e-007
220000.	9.56000e-015	3.20850e-007	2.50800e-007
225000.	6.09000e-015	3.05670e-007	2.44150e-007
230000.	3.89000e-015	2.91870e-007	2.37500e-007
235000.	2.49000e-015	2.78760e-007	2.30850e-007
240000.	1.59000e-015	2.67030e-007	2.25150e-007
245000.	1.02000e-015	2.55990e-007	2.19450e-007
250000.	6.55000e-016	2.44950e-007	2.14700e-007
255000.	4.21000e-016	2.35290e-007	2.09000e-007
260000.	2.71000e-016	2.25630e-007	2.04250e-007
265000.	1.74000e-016	2.17350e-007	2.00450e-007
270000.	1.12000e-016	2.09070e-007	1.95700e-007
275000.	7.23000e-017	2.01480e-007	1.90950e-007
280000.	4.66000e-017	1.93890e-007	1.87150e-007
285000.	3.01000e-017	1.86990e-007	1.83350e-007
290000.	1.94000e-017	1.80780e-007	1.79550e-007
295000.	1.26000e-017	1.74570e-007	1.76700e-007

Time (yr)	Cm-245 (Ci/m^3)	Np-237 (Ci/m^3)	U-233 (Ci/m^3)
300000.	8.12000e-018	1.68360e-007	1.72900e-007
305000.	5.25000e-018	1.62840e-007	1.69100e-007

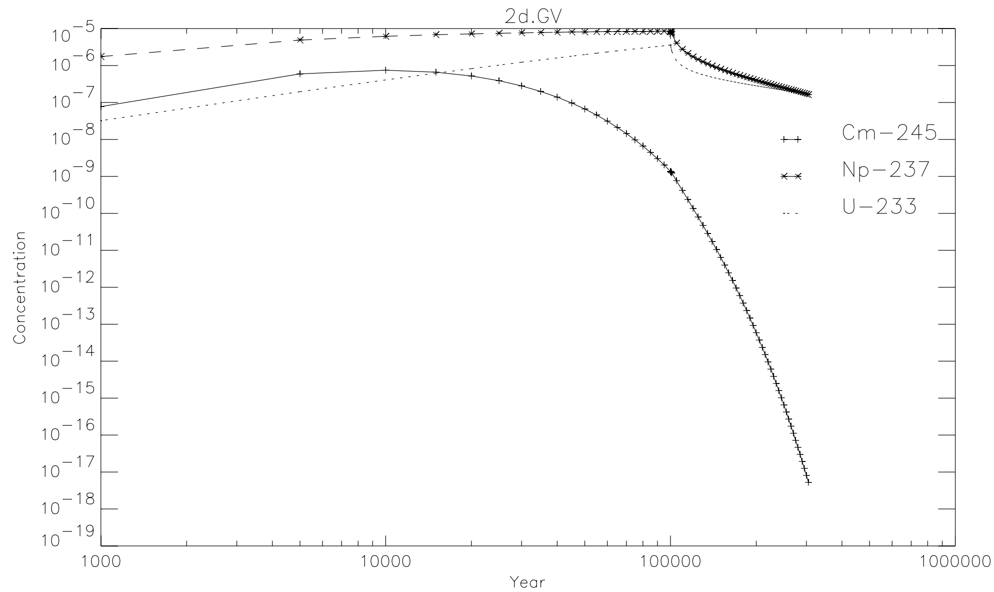

Figure 9. Fracture contaminant breakthrough (Ci/m^3) for the 1-D fractured media simulation for problem 9.1.

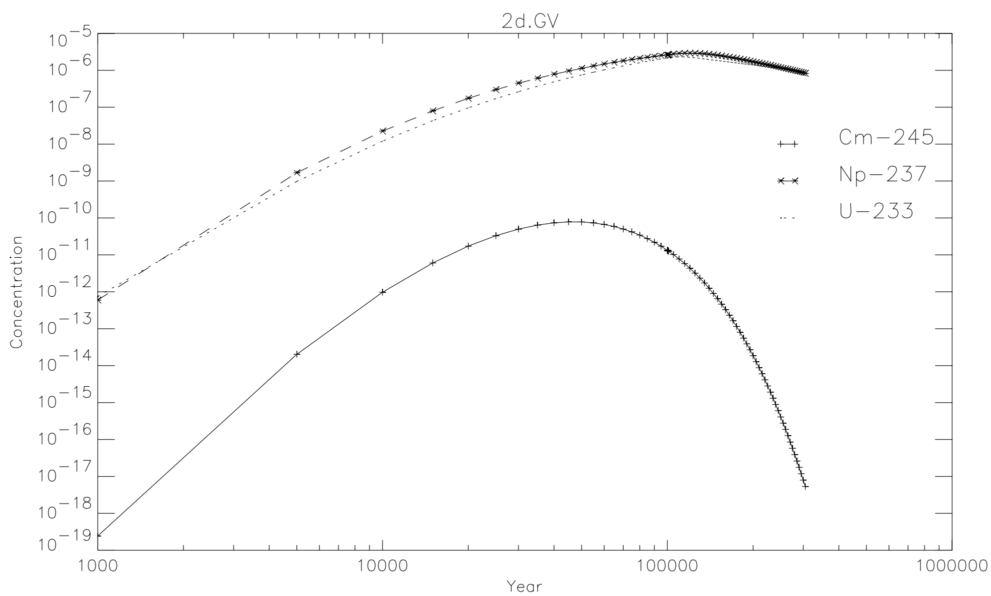

Figure 10. Matrix contaminant breakthrough (Ci/m^3) for the 1-D fractured media simulation for problem 9.1.

7 PROBLEM 8.4 THREE-DIMENSIONAL TRANSPORT FROM A HYPOTHETICAL BASALT REPOSITORY

7.1 Problem Description and Objectives

This problem is a hypothetical basalt repository located in a four sided basin. An upper and lower aquifer are separated by a thick aquitard. The lower aquifer is recharged at the basin's southern margin and flows to the upper aquifer through a crush zone of high permeability located at the northern margin of the basin. The upper aquifer discharges to a river of constant head located on the western margin of the basin. A highly permeable zone resulting from the river's former course is present near the river. The basalt repository is located in the center of the aquitard separating the aquifers. Most flow from the lower to upper aquifer occurs through the crush zone, but a small amount flows upward through the aquitard and repository. The river is the final receptor of any contamination leaving the repository. The test assumptions include:

- The hydraulic properties are isotropic.
- Flow is steady-state.
- The aquifers are confined.
- The river behaves as a constant head boundary.
- Sorption is in equilibrium.
- The simulation is isothermal

The objective of this problem is to test a code ability to simulate three-dimensional flow and transport of a three member radionuclide chain. The required output is the total discharge in Ci/yr to the river for each radiouclide versus time.

7.2 TETRAD Simulation

The problem was discretized as three-dimensional 20x10x11 grid. The simulation used uniform 500m x 500m horizontal grid discretization and a non-uniform vertical discretization. The grid was identical to the USGS3D grid provided in the problem statement except for the central layers. An additional 10m thick layer was defined in the aquitard center and the layers above and below this layer were reduced by 5m each. This was needed because the 'BVMULT' source multiplication approach requires the source be located within model gridblocks. The simulation approach used to define the repository source term is identical to the approach used in problems 8.1 and 8.2. The source area was defined in the 10m thick central layer within the aquitard. Table 13 presents the TETRAD simulation parameters.

The lower aquifer's recharge zone at the basin's southern margin must be isolated from the upper aquifer and aquitard. The TETRAD 'TMULT' option was used to set the interblock transmissibility between the lower aquifer's recharge zone and these two flow units to zero. This effectively makes a no-flow boundary at the grid block vertical interfaces. The simulation was assumed to be confined and a one atmosphere confining pressure was used to ensure the model remained fully saturated everywhere. The one atmosphere confining pressure was also added to the river boundary condition. No numerical problems were encountered and the tracer mass balance was very good at approximately 1.e-10. The simulations was run to 1.e+6 years. No substantial amount of the contaminants from the repository will arrive at the river during the simulation period because of the following reasons:

- The total recharge water volume was approximately 5.e+10 m^3 after 1.e+6 years of recharge and the pore volume of the aquifer system is approximately 1.e+9 m^3. This will allow approximately 50 pore volumes to pass through the aquifer system during the simulation period.
- The contaminant retardation values are large. The smallest basalt retardation factor was 300 for the U-234

and will require several million years to reach the river.

- The longest lived nuclide was U-234 and the half-life was 2.4e+5 years and will result in radioactive decay removing the contaminant before breakthrough to the river.
- Most recharge flow will bypasses the repository located in the aquitard because recharge to the upper aquifer occurs mostly through the crush zone located north of the repository.

Figures 11 and 12 illustrate the aquifer pressure head in the upper aquifer and lower aquifer, respectively. The one atmosphere confining pressure has been subtracted from the pressure in Figures 11 and 12. Figure 13 illustrates the horizontal concentration (Ci/m^3) at the aquifer surface after 1.e+6 years and Figure 14 illustrates the east-west vertical concentration through the repository center after 1.e+6 years. These figures show the contaminant concentrations at the river remain nearly zero after 1.e+6 years.

Table 13. TETRAD simulation parameters for problem 8.4.

Parameter	Value
Upper Aquifer Porosity	0.01
Upper Aquifer Permeability (mD)	10.
Lower Aquifer Porosity	0.01
Lower Aquifer Permeability (mD)	10.
Aquitard Porosity	0.01
Aquitard Permeability (mD)	10.
Crush Zone Porosity	0.01
Crush Zone Permeability (mD)	0.01
River Bed Porosity	10.
River Bed Permeability (mD)	10.
Liquid Density (Kg/m^3)	1000
Viscosity (mPa S)	1.17
Temperature (degree C)	15.
Particle Density (Kg/m^3)	2650.
Longitudinal Dispersivity (m)	50.
Transverse Dispersivity (m)	5.

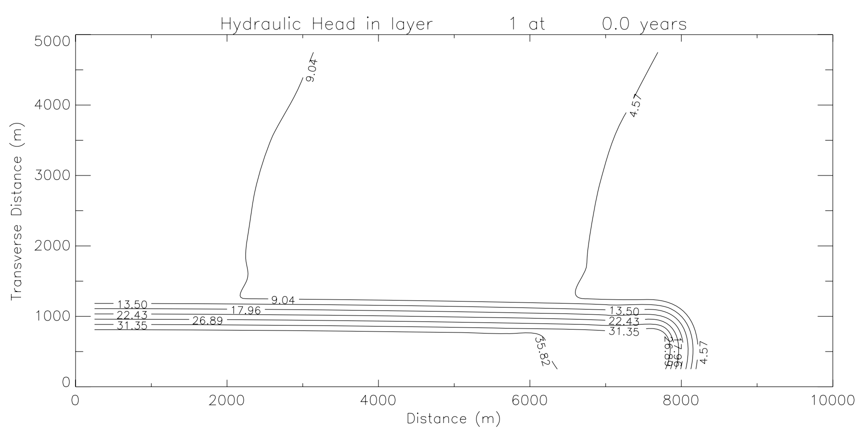

Figure 11. Upper aquifer pressure head (m) for problem 8.4.

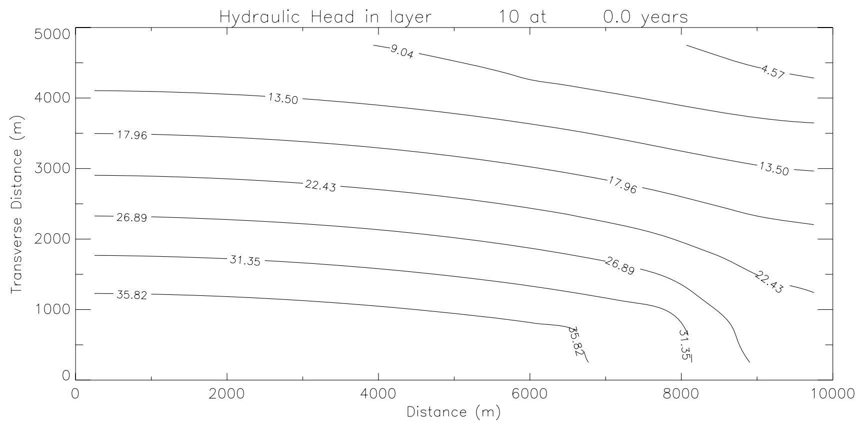

Figure 12. Lower aquifer pressure head (m) for problem 8.4.

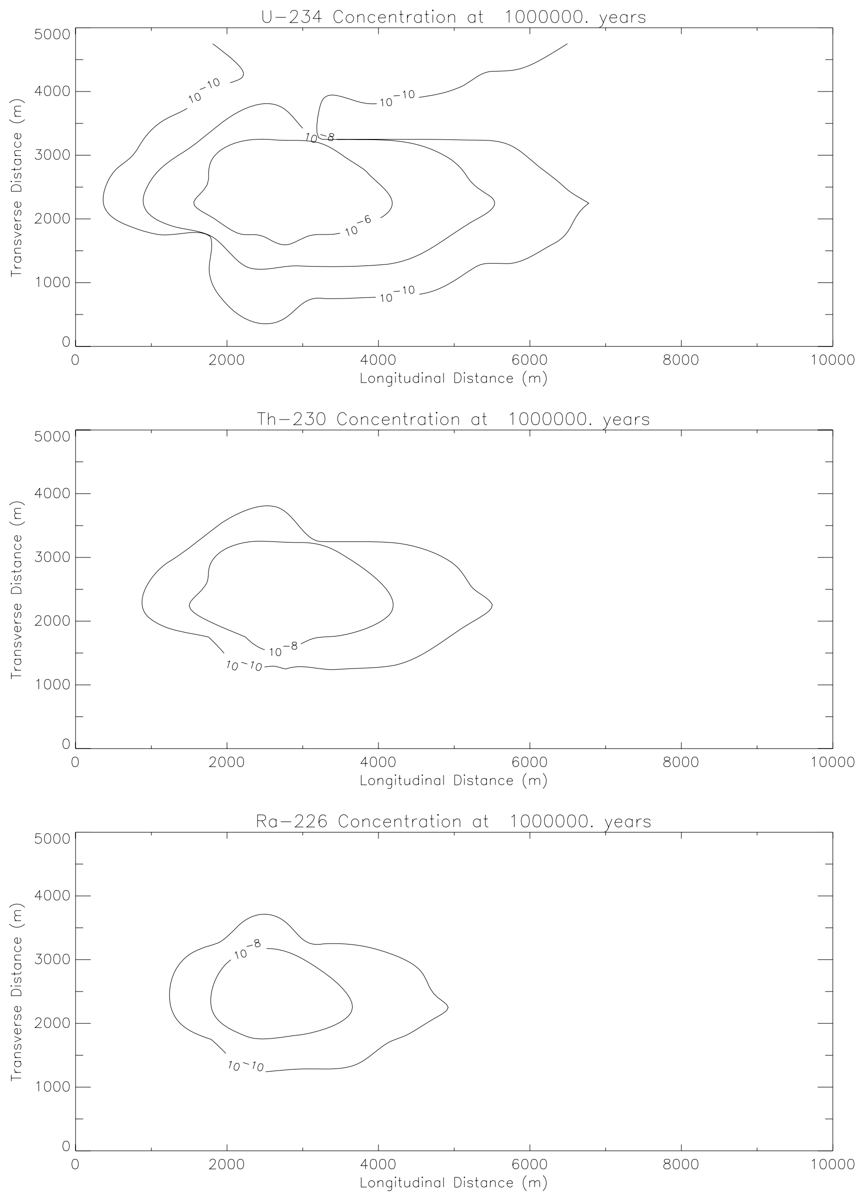

Figure 13. Horizontal normalized concentration in the upper aquifer after 1.e+5 years for problem 8.4.

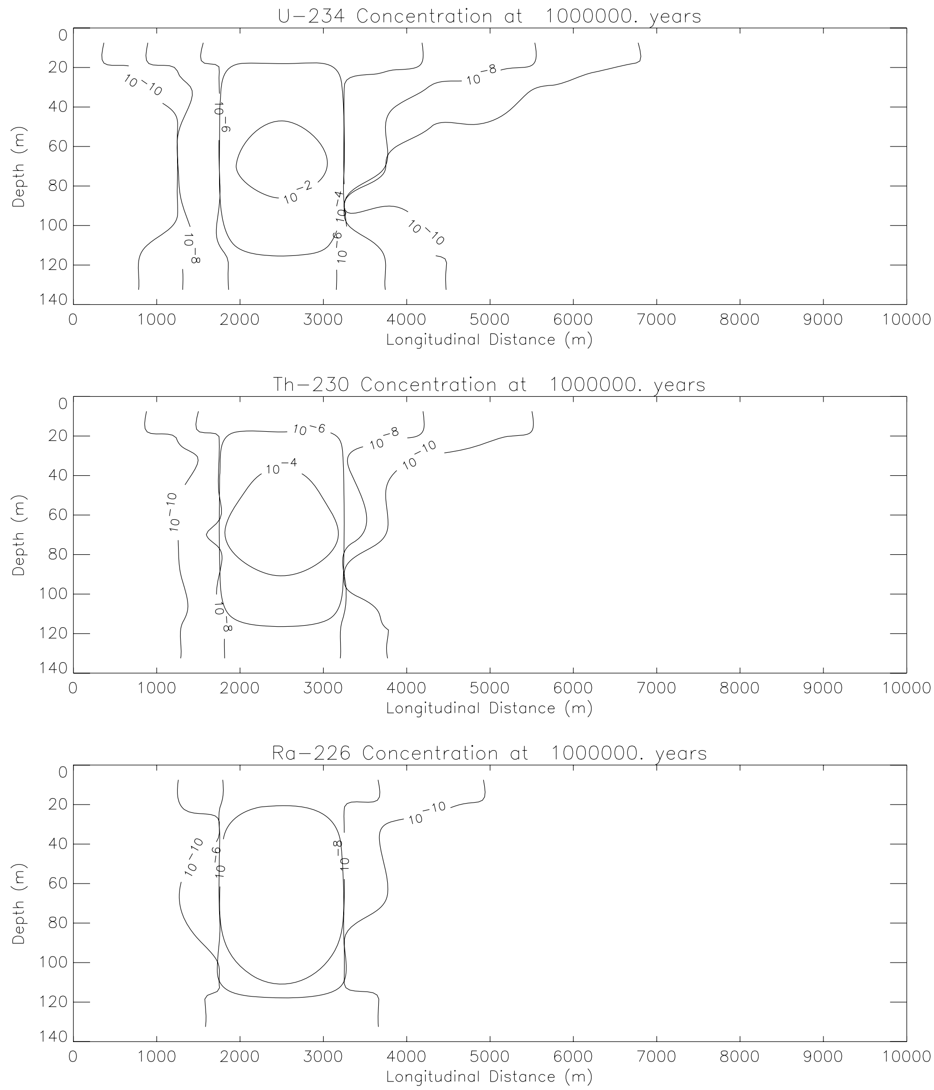

Figure 14. East-West vertical normalized concentration through the repository center after 1.e+5 years for problem 8.4.

8 PROBLEM 10.1: ONE-DIMENSIONAL HYDRODYNAMIC DISPERSION DURING ADSORPTION OF WATER BY SOIL

8.1 Problem Description and Objectives

This problem simulates unsaturated horizontal water flow and solute transport in a tube of soil. The dispersion coefficient is assumed to be only a function of moisture content. Hydrodynamic dispersion due to the water velocity is neglected.The soil has an uniform initial moisture content and solute concentration. At time zero, the upstream boundary is subject to saturated conditions and a higher solute concentration. The test assumptions include:

- Hydraulic and transport properties are constant.
- Moisture and matric potential characteristic curves are non-hysteretic.
- Water velocity is slow and hydrodynamic dispersion can be neglected.
- Diffusion coefficient is a function of moisture content.
- Flow and transport are one-dimensional.

The objective of this problem is to test the code's ability to simulate unsaturated flow and transport and identify problems between flow and transport code assumptions. The required output is the concentration and moisture content versus distance at times of 0.01, 0.06, and 0.11 days.

8.2 TETRAD Simulation

This problem is well suited for the TETRAD code because it is a multiphase and multicomponent simulator. The flow and transport equations are linked in the TETRAD simulator and there is no conflicting assumptions between the flow and solute transport solutions. The 20 cm soil column was discretized using 250 0.0008 m grid blocks. The upstream boundary condition was parameterized using the 'AQUIFER' keyword (Dirichlet boundary condition) with the pressure specified in the water phase. The constitutive relationships for matric potential and hydraulic conductivity were parameterized using the 'RELANAL' keyword (analytic relative permeability function). Identical forms of the constitutive functions were created by setting the exponential terms in the TETRAD functions to 1. TETRAD simulates solute diffusion in unsaturated flow identical to the benchmark analytical solution if the tortuosity parameter is set to 1. The TETRAD simulation parameters are presented in Table 14.

No numerical problems were encountered and the tracer mass balance was very good at 1.e-6. Dispersion control was implemented with the TETRAD 'DISC' keyword and the water dispersion control parameter set to a value of 1.5. Implementing dispersion control makes the solution more explicit and the 'NORM' keyword was used to allow a 0.06 fractional change in the mole fraction over a Newton iteration. This is analogous to restricting the time step and prevents simulation overshoot or undershoot. The simulated soil moisture content versus time is presented in Table 15 and illustrated in Figure 15. The simulated solute concentration versus time is presented in Table 16 and illustrated in Figure 16.

Table 14. TETRAD simulation parameters for problem 10.1.

Parameter	Value
Soil Porosity	0.45
Soil Permeability (mD)	14.40
Residual Saturation	0.3333
Residual Capillary Pressure (KPa)	9.81

Parameter	Value
Initial Saturation	0.4444
Initial Capillary Pressure (KPa)	8.18
TETRAD APCOW Parameter (KPa)	14.71
TETRAD BPCOW Parameter	1.
TETRAD A Parameter	1.
TETRAD AN Parameter	1.
Liquid Density (Kg/m^3)	1000.
Viscosity (mPa S)	1.0
Temperature (degree C)	15.
Diffusion Coefficient (m^2/day)	1.e-4
Tortuosity	1.0

Table 15. Moisture content versus distance at 0.01, 0.06, and 0.11 days for problem 10.1.

Distance (m)	Volumetric Moisture Content at 0.01 days	Volumetric Moisture Content at 0.06 days	Volumetric Moisture Content at 0.11 days
0.000400000	0.415996	0.437277	0.441208
0.00120000	0.410571	0.435101	0.439613
0.00200000	0.405083	0.432913	0.438010
0.00280000	0.399532	0.430711	0.436400
0.00360000	0.393920	0.428497	0.434783
0.00440000	0.388250	0.426270	0.433158
0.00520000	0.382523	0.424030	0.431527
0.00600000	0.376742	0.421777	0.429888
0.00680000	0.370911	0.419512	0.428243
0.00760000	0.365032	0.417235	0.426590
0.00840000	0.359110	0.414945	0.424930
0.00920000	0.353148	0.412642	0.423263
0.0100000	0.347151	0.410328	0.421589
0.0108000	0.341125	0.408001	0.419908
0.0116000	0.335074	0.405661	0.418220
0.0124000	0.329007	0.403311	0.416525
0.0132000	0.322928	0.400948	0.414823
0.0140000	0.316847	0.398574	0.413114
0.0148000	0.310772	0.396188	0.411399
0.0156000	0.304713	0.393791	0.409677
0.0164000	0.298680	0.391383	0.407947
0.0172000	0.292684	0.388964	0.406212
0.0180000	0.286740	0.386534	0.404470
0.0188000	0.280860	0.384094	0.402721
0.0196000	0.275061	0.381643	0.400966

Distance (m)	Volumetric Moisture Content at 0.01 days	Volumetric Moisture Content at 0.06 days	Volumetric Moisture Content at 0.11 days
0.0204000	0.269359	0.379182	0.399204
0.0212000	0.263773	0.376711	0.397436
0.0220000	0.258322	0.374231	0.395662
0.0228000	0.253027	0.371740	0.393881
0.0236000	0.247910	0.369242	0.392095
0.0244000	0.242995	0.366733	0.390302
0.0252000	0.238303	0.364216	0.388503
0.0260000	0.233860	0.361692	0.386698
0.0268000	0.229684	0.359158	0.384888
0.0276000	0.225798	0.356618	0.383071
0.0284000	0.222216	0.354070	0.381249
0.0292000	0.218952	0.351515	0.379422
0.0300000	0.216012	0.348953	0.377588
0.0308000	0.213397	0.346385	0.375750
0.0316000	0.211100	0.343812	0.373905
0.0324000	0.209110	0.341233	0.372056
0.0332000	0.207408	0.338649	0.370202
0.0340000	0.205971	0.336061	0.368343
0.0348000	0.204772	0.333469	0.366479
0.0356000	0.203784	0.330873	0.364610
0.0364000	0.202979	0.328275	0.362736
0.0372000	0.202329	0.325674	0.360859
0.0380000	0.201809	0.323072	0.358976
0.0388000	0.201397	0.320468	0.357089
0.0396000	0.201072	0.317865	0.355198
0.0404000	0.200818	0.315261	0.353304
0.0412000	0.200621	0.312659	0.351405
0.0420000	0.200468	0.310058	0.349503
0.0428000	0.200351	0.307460	0.347598
0.0436000	0.200261	0.304865	0.345689
0.0444000	0.200193	0.302274	0.343777
0.0452000	0.200141	0.299688	0.341862
0.0460000	0.200102	0.297109	0.339944
0.0468000	0.200072	0.294536	0.338024
0.0476000	0.200050	0.291972	0.336101
0.0484000	0.200034	0.289416	0.334176
0.0492000	0.200021	0.286871	0.332249
0.0500000	0.200012	0.284337	0.330320
0.0508000	0.200006	0.281815	0.328390
0.0516000	0.200001	0.279308	0.326459
0.0524000	0.199997	0.276815	0.324526

Distance (m)	Volumetric Moisture Content at 0.01 days	Volumetric Moisture Content at 0.06 days	Volumetric Moisture Content at 0.11 days
0.0532000	0.199994	0.274339	0.322593
0.0540000	0.199992	0.271881	0.320659
0.0548000	0.199991	0.269441	0.318725
0.0556000	0.199989	0.267023	0.316791
0.0564000	0.199989	0.264627	0.314857
0.0572000	0.199988	0.262255	0.312925
0.0580000	0.199988	0.259909	0.310992
0.0588000	0.199988	0.257589	0.309061
0.0596000	0.199987	0.255299	0.307132
0.0604000	0.199987	0.253040	0.305204
0.0612000	0.199987	0.250813	0.303279
0.0620000	0.199987	0.248621	0.301356
0.0628000	0.199987	0.246465	0.299437
0.0636000	0.199987	0.244348	0.297521
0.0644000	0.199987	0.242270	0.295608
0.0651999	0.199987	0.240235	0.293700
0.0659999	0.199987	0.238243	0.291797
0.0667999	0.199986	0.236298	0.289898
0.0675999	0.199986	0.234400	0.288005
0.0683999	0.199986	0.232551	0.286118
0.0691999	0.199986	0.230754	0.284237
0.0699999	0.199986	0.229009	0.282364
0.0707999	0.199986	0.227318	0.280498
0.0715999	0.199986	0.225683	0.278640
0.0723999	0.199986	0.224105	0.276790
0.0731999	0.199986	0.222585	0.274949
0.0739999	0.199986	0.221124	0.273118
0.0747999	0.199986	0.219722	0.271298
0.0755999	0.199986	0.218381	0.269488
0.0763999	0.199986	0.217100	0.267690
0.0771999	0.199986	0.215880	0.265904
0.0779999	0.199986	0.214721	0.264131
0.0787999	0.199986	0.213621	0.262371
0.0795999	0.199986	0.212581	0.260626
0.0803999	0.199986	0.211600	0.258895
0.0811999	0.199986	0.210676	0.257179
0.0819999	0.199986	0.209809	0.255481
0.0827999	0.199986	0.208997	0.253799
0.0835999	0.199986	0.208237	0.252135
0.0843999	0.199986	0.207530	0.250488
0.0851999	0.199986	0.206872	0.248862

Distance (m)	Volumetric Moisture Content at 0.01 days	Volumetric Moisture Content at 0.06 days	Volumetric Moisture Content at 0.11 days
0.0859999	0.199985	0.206262	0.247256
0.0867999	0.199985	0.205696	0.245670
0.0875999	0.199985	0.205174	0.244106
0.0883999	0.199985	0.204693	0.242564
0.0891999	0.199985	0.204250	0.241046
0.0899999	0.199985	0.203844	0.239551
0.0907999	0.199985	0.203472	0.238081
0.0915999	0.199985	0.203131	0.236636
0.0923999	0.199985	0.202820	0.235218
0.0931999	0.199985	0.202537	0.233826
0.0939999	0.199985	0.202279	0.232462
0.0947999	0.199985	0.202045	0.231127
0.0955999	0.199985	0.201834	0.229820
0.0963999	0.199985	0.201641	0.228543
0.0971999	0.199985	0.201468	0.227296
0.0979999	0.199985	0.201311	0.226080
0.0987999	0.199985	0.201169	0.224895
0.0995999	0.199985	0.201042	0.223742
0.100400	0.199985	0.200928	0.222621

Table 16. Normalized concentration versus distance at 0.01, 0.06, and 0.11 days for problem 10.1.

Distance (m)	Solute Concentration at 0.01 days	Solute Concentration at 0.06 days	Solute Concentration at 0.11 days
0.000400000	1.00000	1.00000	1.00000
0.00120000	1.00000	1.00000	1.00000
0.00200000	1.00000	1.00000	1.00000
0.00280000	0.999000	1.00000	1.00000
0.00360000	0.996000	1.00000	1.00000
0.00440000	0.991000	1.00000	1.00000
0.00520000	0.978000	1.00000	1.00000
0.00600000	0.952000	1.00000	1.00000
0.00680000	0.900000	1.00000	1.00000
0.00760000	0.812000	1.00000	1.00000
0.00840000	0.675000	1.00000	1.00000
0.00920000	0.489000	1.00000	1.00000
0.0100000	0.306000	1.00000	1.00000
0.0108000	0.197000	1.00000	1.00000
0.0116000	0.142000	0.999000	1.00000
0.0124000	0.116000	0.999000	1.00000

Distance (m)	Solute Concentration at 0.01 days	Solute Concentration at 0.06 days	Solute Concentration at 0.11 days
0.0132000	0.106000	0.998000	1.00000
0.0140000	0.102000	0.996000	1.00000
0.0148000	0.101000	0.994000	1.00000
0.0156000	0.100000	0.989000	1.00000
0.0164000	0.100000	0.981000	1.00000
0.0172000	0.100000	0.970000	0.999000
0.0180000	0.100000	0.953000	0.999000
0.0188000	0.100000	0.928000	0.998000
0.0196000	0.100000	0.894000	0.997000
0.0204000	0.100000	0.850000	0.995000
0.0212000	0.100000	0.794000	0.993000
0.0220000	0.100000	0.726000	0.989000
0.0228000	0.100000	0.650000	0.983000
0.0236000	0.100000	0.568000	0.975000
0.0244000	0.100000	0.486000	0.964000
0.0252000	0.100000	0.410000	0.949000
0.0260000	0.100000	0.342000	0.930000
0.0268000	0.100000	0.283000	0.905000
0.0276000	0.100000	0.235000	0.874000
0.0284000	0.100000	0.197000	0.837000
0.0292000	0.100000	0.168000	0.794000
0.0300000	0.100000	0.147000	0.746000
0.0308000	0.100000	0.131000	0.692000
0.0316000	0.100000	0.120000	0.636000
0.0324000	0.100000	0.113000	0.578000
0.0332000	0.100000	0.108000	0.521000
0.0340000	0.100000	0.105000	0.465000
0.0348000	0.100000	0.103000	0.412000
0.0356000	0.100000	0.102000	0.362000
0.0364000	0.100000	0.101000	0.317000
0.0372000	0.100000	0.101000	0.278000
0.0380000	0.100000	0.100000	0.243000
0.0388000	0.100000	0.100000	0.214000
0.0396000	0.100000	0.100000	0.189000
0.0404000	0.100000	0.100000	0.169000
0.0412000	0.100000	0.100000	0.152000
0.0420000	0.100000	0.100000	0.139000
0.0428000	0.100000	0.100000	0.129000
0.0436000	0.100000	0.100000	0.122000
0.0444000	0.100000	0.100000	0.116000
0.0452000	0.100000	0.100000	0.111000

Distance (m)	Solute Concentration at 0.01 days	Solute Concentration at 0.06 days	Solute Concentration at 0.11 days
0.0460000	0.100000	0.100000	0.108000
0.0468000	0.100000	0.100000	0.106000
0.0476000	0.100000	0.100000	0.104000
0.0484000	0.100000	0.100000	0.103000
0.0492000	0.100000	0.100000	0.102000
0.0500000	0.100000	0.100000	0.101000
0.0508000	0.100000	0.100000	0.101000
0.0516000	0.100000	0.100000	0.101000
0.0524000	0.100000	0.100000	0.100000
0.0532000	0.100000	0.100000	0.100000

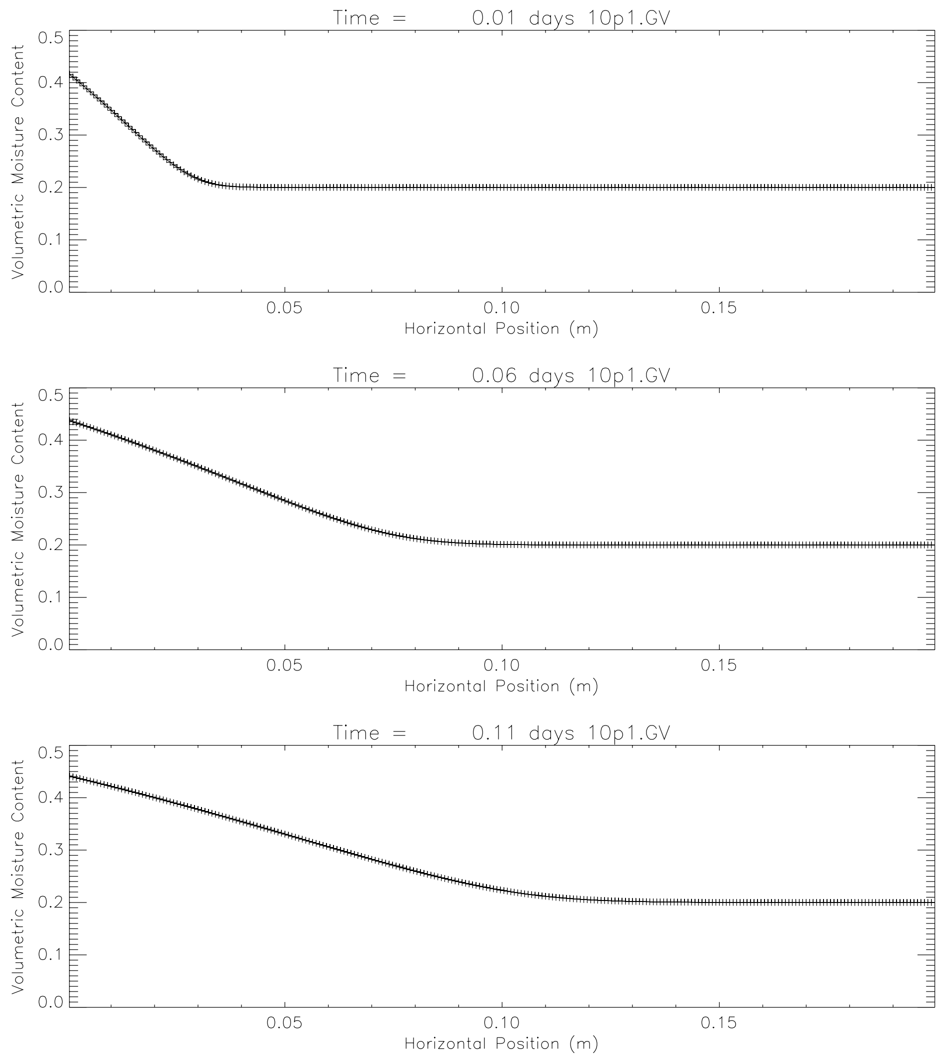

Figure 15. Moisture content versus distance at 0.01, 0.06, and 0.11 days for problem 10.1.

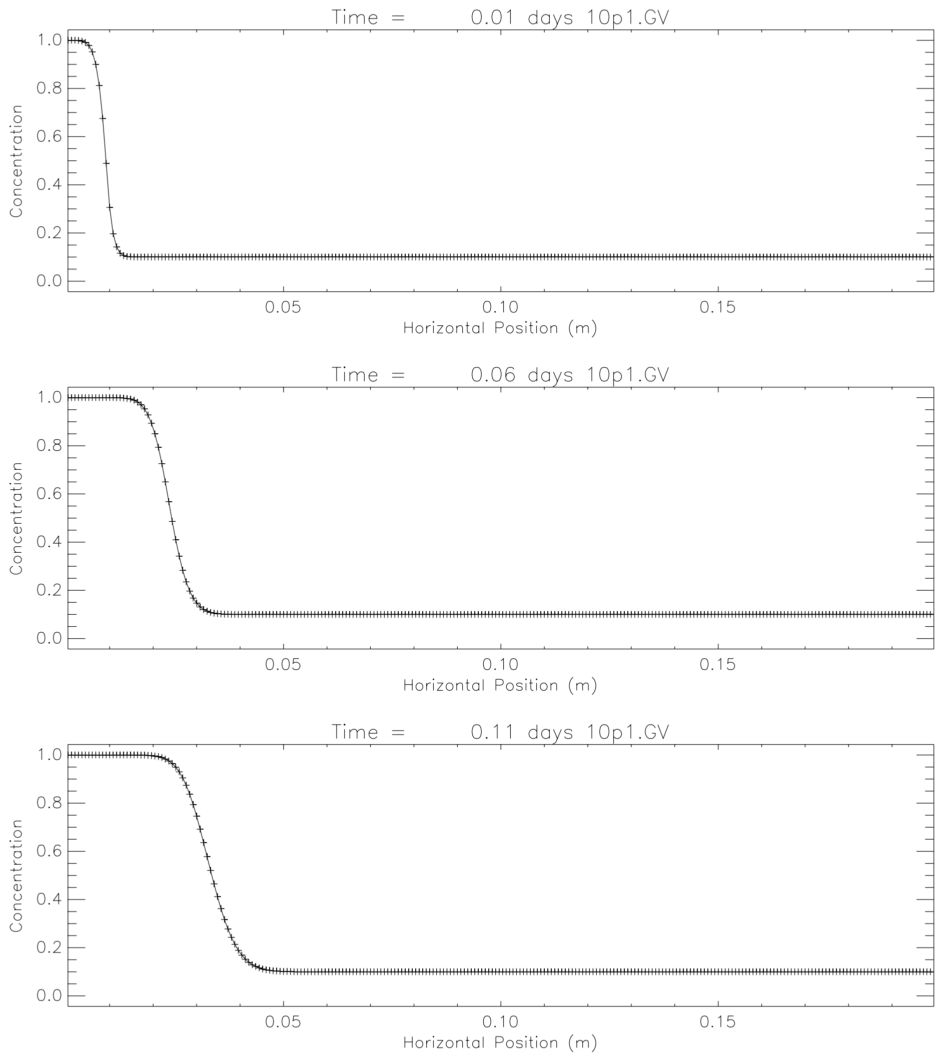

Figure 16. Normalized concentration versus distance at 0.01, 0.06, and 0.11 days for problem 10.1.

9 PROBLEM 10.2: TWO-DIMENSIONAL FLOW AND TRANSPORT IN THE UNSATURATED ZONE

9.1 Problem Description and Objectives

This problem simulates unsaturated horizontal water flow and solute transport in two-dimensional vertical rectangle of soil. The problem has uniform initial conditions and the upper left region is subjected to an increase in capillary pressure and solute concentration. A wetting and solute front moves through the rectangle over time. The problem assumptions include:

- The fluid is slightly compressible.
- The flow is two-dimensional.
- Porosity, saturated hydraulic conductivity, and specific storage do not vary with time.
- Relative permeability is a function of matric potential.

The purpose of this problem is to test the code's accuracy in simulating two-dimensional unsaturated flow and transport with decay and sorption. The required output the normalized concentration versus height at x = 3 cm for times of 0.165 and 0.508 days; and the normalized concentration versus distance along the x-axis at the domain top (z = 10 cm) for times of 0.053, 0.165, and 0.508 days.

9.2 TETRAD Simulation

The simulation approach for this problem was nearly identical to the approach used in problem 10.1. The soil moisture characteristics are identical to those used in problem 10.1. The difference between problem 10.2 and problem 10.1 is that problem 10.2 also considers hydrodynamic dispersion, retardation, and solute decay. The TETRAD parameters for problem 10.2 are provided in Table 17. The problem statement assumed the fluid is slightly compressible, but a value was not specified. The TETRAD simulation assumed the fluid compressibility to be 5.e-7 (1/KPa).

The 15 cm long and 10 cm high simulation domain used a uniform 0.5 cm horizontal and vertical grid block size. The water and solute boundary conditions in the upper left of the model domain were specified by setting boundary cell saturation and concentration using the 'BVMULT' keyword. This multiplied grid block volume by a factor of 1e+10 and maintained constanst water phase pressure was maintained at each boundary node cell center using the boundary condition Ψ = 6-z for z = 6 to 10 cm. The normalized solute concentration at the boundary was specified as a small uniform value (1.e-6). The small concentration was needed to prevent pressure changes resulting from mass (and volume) transferring from the aqueous phase to the sorbed phase (see Section 1.1.2). Gas phase "AQUIFER" keyword boundary were attached around the entire perimeter of the simulation domain and set the gas phase pressure to 101.3 KPa. This was needed to allow the gaseous phase to escape and prevent excessive gas phase pressure build up as water entered the simulation domain. The solution results were scaled back to a normalized concentration of 1.0 at the boundary.

The benchmark problem statement assumed retardation was independent of saturation. This is consistent with the sorption formulation in TETRAD (i.e., the fraction adsorbed equals the product of the sorption coefficient, concentration and saturation). However, this is not consistent with the generally accepted relationship for unsaturated transport in the literature, which assumes retardation increases with decreasing saturation because the ratio of rock mass to water volume increases with lower saturations.

No numerical problems were encountered and the tracer mass balance was very good at 1.e-5. The relative concentration versus height at x = 3 cm at 0.053, 0.165, and 0.508 days is provided in Table 18. The model grid block centers occurred at x=2.75 cm and x= 3.25 cm, and the concentration provided in Table 18 is the average of the two locations. Table 19 presents the relative concentration versus length at z = 9.75 cm at 0.053, 0.165, and 0.508 days. The discrete nature of finite difference numerical model grid block sizes do allow concentration calculation at the domain boundary and 9.75 cm represents the grid block center of upper most row. Figures 17 illustrates the saturation profiles at 0.053, 0.165, and 0.508 days. Figures 18, 19 and 20 illustrate the concentration profiles at 0.053, 0.165, and 0.508 days; respectively.

Table 17. TETRAD simulation parameters for problem 10.2.

Parameter	Value
Soil Porosity	0.45
Soil Permeability (mD)	14.40
Residual Saturation	0.3333
Residual Capillary Pressure (KPa)	9.81
Initial Saturation	0.4
Initial Capillary Pressure (KPa)	8.826
TETRAD APCOW Parameter (KPa)	14.71
TETRAD BPCOW Parameter	1.
TETRAD A Parameter	1.
TETRAD AN Parameter	1.
Liquid Density (Kg/m^3)	1000.
Viscosity (mPa S)	1.0
Temperature (degree C)	15.
Liquid Compressibility (1/KPa)	5.e-7
Diffusion Coefficient (m^2/day)	1.e-6
Tortuosity	1.0
Longitudinal Dispersivity (m)	0.01
Transverse Dispersivity (m)	0.01
Sorption Coefficient (mL/g)	0.3087
Decay Coefficient (1/year)	0.36525

Table 18. Relative concentration versus height at x = 3 cm at 0.053, 0.165, and 0.508 days for problem 10.2.

Height (cm)	Time (days) 0.053	Time (days) 0.165	Time (days) 0.508
0.250000	1.49041e-008	0.00211937	0.0541969
0.750000	5.28875e-007	0.00593094	0.0794062
1.25000	9.12781e-006	0.0151094	0.128500
1.75000	9.21750e-005	0.0326438	0.197969
2.25000	0.000603281	0.0617406	0.281844
2.75000	0.00275156	0.104525	0.371719
3.25000	0.00921156	0.159906	0.460781
3.75000	0.0236656	0.224625	0.542625
4.25000	0.0484594	0.291344	0.612656
4.75000	0.0811969	0.353437	0.670469
5.25000	0.115322	0.404906	0.714469
5.75000	0.144594	0.443750	0.746469

Height (cm)	Time (days) 0.053	Time (days) 0.165	Time (days) 0.508
6.25000	0.166250	0.469969	0.768656
6.75000	0.178469	0.485375	0.782844
7.25000	0.184469	0.492375	0.790438
7.75000	0.185062	0.493562	0.794625
8.25000	0.182844	0.490344	0.795219
8.75000	0.179625	0.485531	0.793813
9.25000	0.176812	0.480719	0.791812
9.75000	0.175406	0.478312	0.790406

Table 19. Relative concentration versus length at z = 9.75 cm at 0.053, 0.165, and 0.508 days for problem 10.2

Length (cm)	Time (days) 0.053	Time (days) 0.165	Time (days) 0.508
0.000000	1.00000	1.00000	0.999000
0.0468750	0.993000	0.997000	0.998000
0.140625	0.977000	0.990000	0.996000
0.328125	0.941000	0.975000	0.991000
0.703125	0.853000	0.939000	0.980000
1.20313	0.699000	0.867000	0.957000
1.70313	0.525000	0.772000	0.926000
2.20313	0.364000	0.662000	0.883000
2.70312	0.233000	0.546000	0.829000
3.20313	0.136000	0.432000	0.764000
3.70312	0.0727000	0.326000	0.689000
4.20312	0.0349000	0.236000	0.608000
4.70312	0.0149000	0.163000	0.523000
5.20312	0.00550000	0.107000	0.439000
5.70312	0.00172000	0.0679000	0.359000
6.20312	0.000439000	0.0414000	0.286000
6.70312	8.69000e-005	0.0243000	0.221000
7.20312	1.26000e-005	0.0138000	0.167000
7.70312	1.24000e-006	0.00757000	0.123000
8.20313	7.75000e-008	0.00398000	0.0880000
8.70313	2.89000e-009	0.00200000	0.0614000
9.20313	6.12000e-011	0.000951000	0.0418000
9.70313	7.25000e-013	0.000424000	0.0276000
10.2031	4.83000e-015	0.000176000	0.0177000
10.7031	1.94000e-017	6.73000e-005	0.0110000
11.2031	5.35000e-020	2.33000e-005	0.00662000
11.7031	1.19000e-022	7.23000e-006	0.00381000
12.2031	2.56000e-025	1.97000e-006	0.00209000
12.7031	5.98000e-028	4.58000e-007	0.00108000

Length (cm)	Time (days) 0.053	Time (days) 0.165	Time (days) 0.508
13.2031	0.000000	8.83000e-008	0.000520000
13.7031	0.000000	1.35000e-008	0.000226000
14.2031	0.000000	1.55000e-009	8.53000e-005
14.7031	0.000000	1.20000e-010	2.59000e-005
15.2031	0.000000	4.90000e-012	5.16000e-006

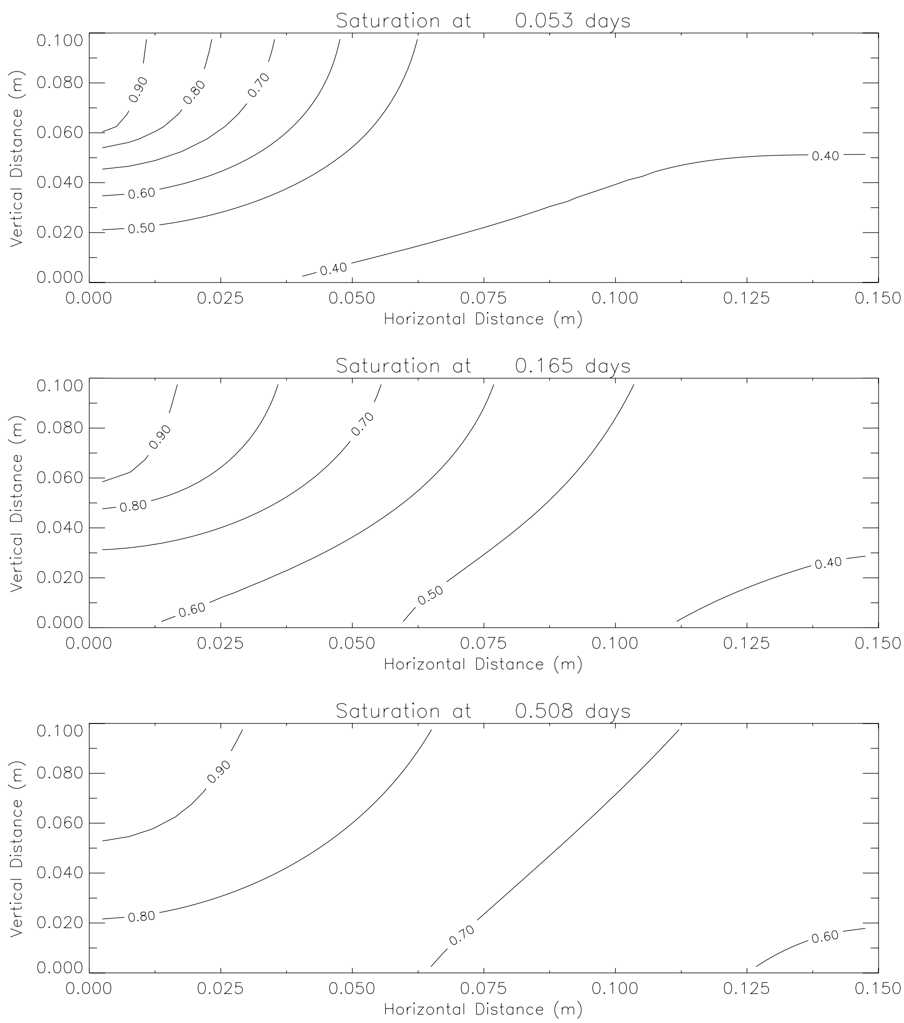

Figure 17. Saturation profile at 0.053, 0.165, and 0.508 days for problem 10.2.

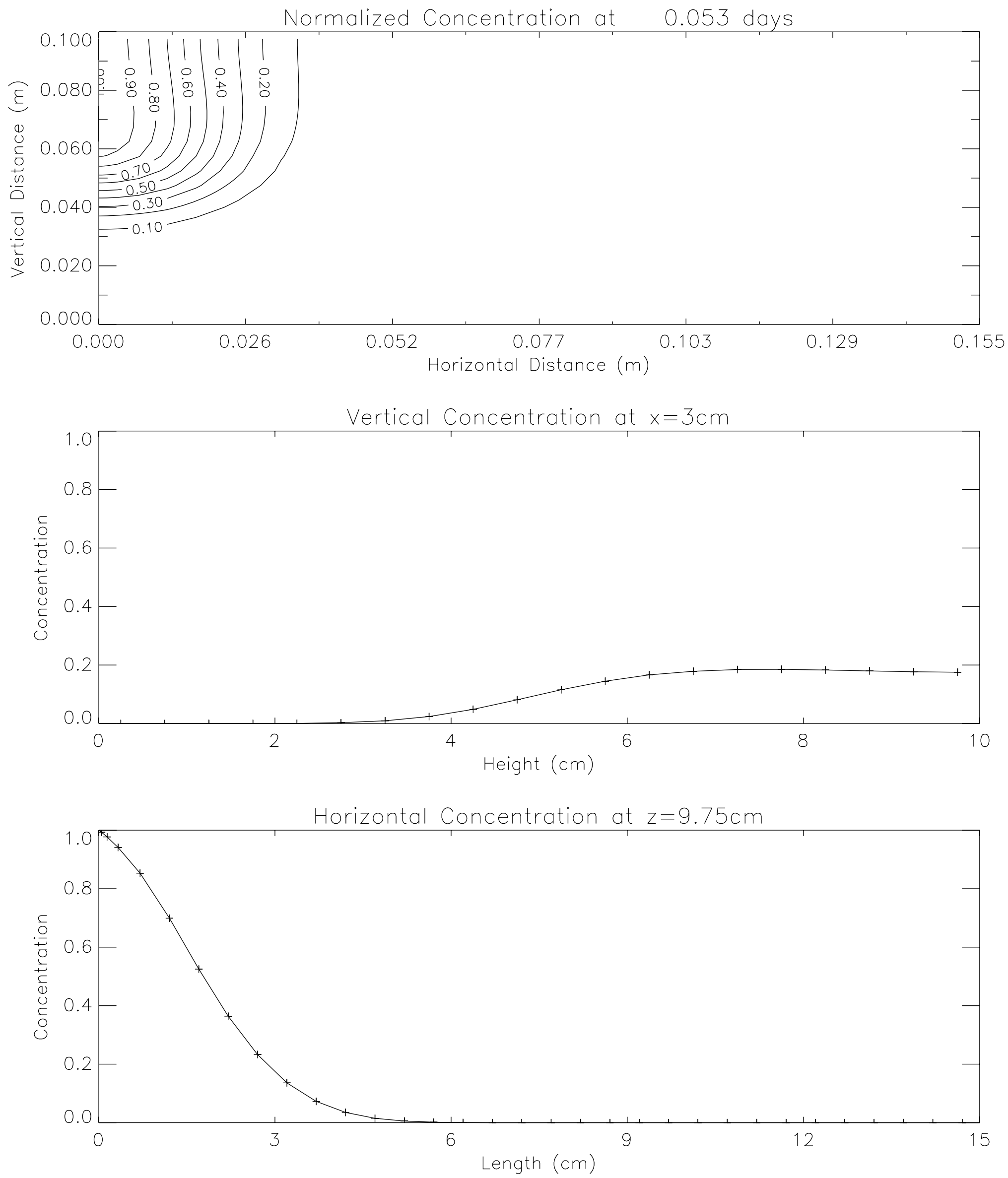

Figure 18. Concentration profile at 0.053 days for problem 10.2.

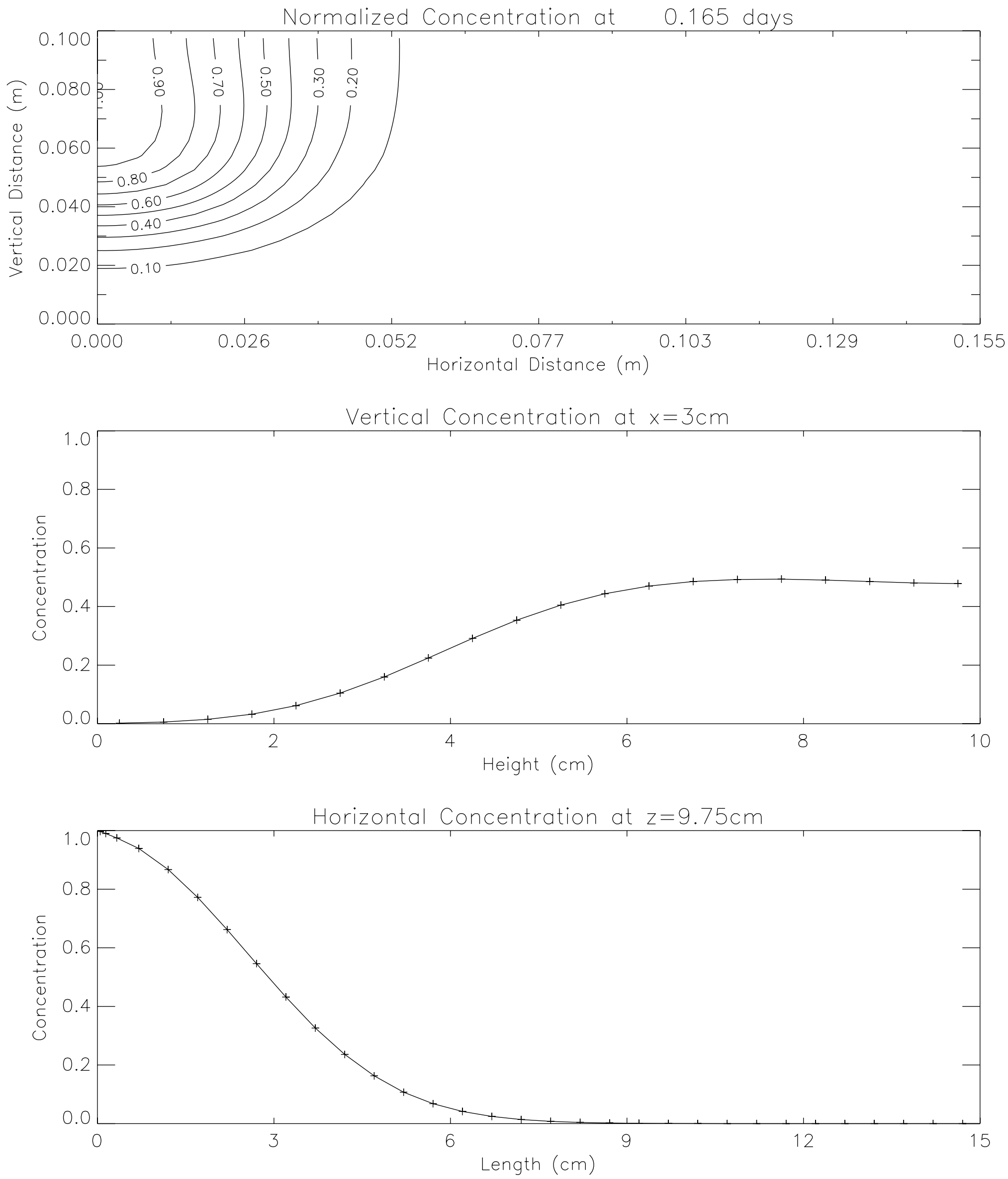

Figure 19. Concentration profile at 0.165 days for problem 10.2.

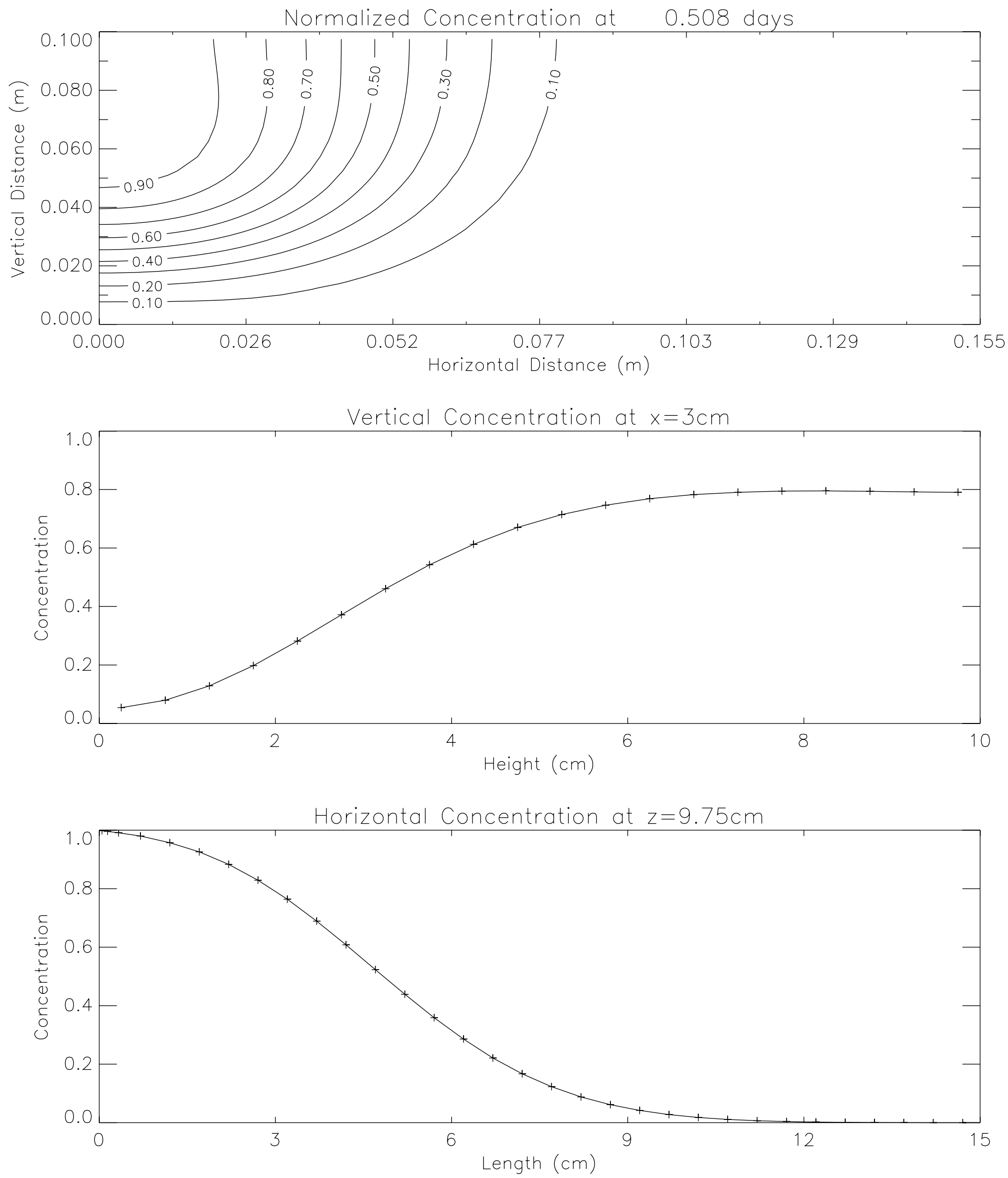

Figure 20. Concentration profile at 0.508 days for problem 10.2.

10 T2VOC BENCHMARK PROBLEM: MULTIPHASE CARBON TETRACHLORIDE TRANSPORT ACROSS A WATERTABLE

10.1 Problem Description and Objectives

This problem required simulating multiphase flow and transport in a combined vadose zone and aquifer domain. This test is three-dimensional and includes a background infiltration, a DNAPL carbon tetrachloride release, a surface flood, and a 4 m head differential across the watertable. The surface flood is transient and occurs over the carbon tetrachloride release site. The simulation domain consists of two material types: Sand and a low permeability clay layer with a gap near the layer center. The problem assumptions include:

- Flow and transport is three-dimensional.
- Porosity, saturated hydraulic conductivity, and specific storage do not vary with time.
- Relative permeability is a function of matric potential.
- Equilibrium partitioning between oleic, aqueous, and gaseous phases.
- Equilibrium sorption.

The objectives of this problem is to test the code's ability to simulate multiphase flow and transport systems. The problem also tests the code's transient flux boundary conditions and the transition from unsaturated to saturated conditions. The required output is vertical concentration plots and concentration time histories at several locations.

10.2 TETRAD Simulation

The TETRAD simulation approach was to establish steady-state initial conditions using with the 1 cm/ year recharge and 4 m head differential across the water table. The simulation was initialized with a 0.6 vadose zone saturation and horizontal water table (static aquifer) and run to steady-state before releasing the carbon tetrachloride. The aquifer flow was simulated using the TETRAD 'AQUIFER' keyword with hydrostatic pressure within the aquifer domain. Atmospheric pressure was set at the simulation surface grid blocks using the 'AQUIFER' keyword and 1 atm of pressure connected to the gaseous phase.

The simulation grid was three-dimensional and included the following discretization: (1) 165 meters in the x-direction (19 grid blocks) with block sizes of 13x5 m, 1x10 m, 2x15 m and 3x20 m blocks; (3) 165 m in the y-direction with the same discretization as the x-direction; and (3) 61 meters in the z-direction (24 layers) with layers of 3x1 m, 4x2 m, 5x1 m, 1x2 m, 1x3 m, and 10x4 m.

The simulation transient boundary conditions are as follows: (1) 0.864 kg/m^2/day of DNAPL carbon tetrachloride is injected from time zero to 365 days at the location of x=8, y=1, and z=3; (2) a 2.738 kg/m^2/day surface flooding event from time 365 to 730 days at the location of x=7 through 8, y=1 through 2, and z=1; and (3) return to background infiltration (1 cm/year) after 730 days. The transient boundary conditions were simulated using the TETRAD 'MFLUX' keyword and the required flux rates for each component. The TETRAD simulation parameters are provided in Table 20.

Slightly different simulation results were expected between the T2VOC and TETRAD models because different moisture characteristics and different phase equilibrium relationships were used in the two models. The TETRAD simulation could not use the identical relative permeability and capillary pressure functions as used by the T2VOC model. The T2VOC model used a relative permeability function provided by Stone's model and capillary pressure function from the Parker modification of the van Genutchen functions (Parker, 1987). TETRAD does not allow the user to specify a non-van Genutchen relative permeability function, if the van Genutchen relations are selected for the capillary pressure function. The van Genutchen relationships were used for both the relative permeability and capillary pressure functions in the TETRAD simulation. The

TETRAD code also uses a different interpretation of the multi-phase van Genutchen relationships. The TETRAD code assigns a single alpha parameter value and scales the capillary pressure calculations by the oil-water, air-oil, and air-water surface tension. The T2VOC code allows different alpha values for gas-NAPL and NAPL-water. The T2VOC problem also used different minimum fluid saturation values for the relative permeability and capillary pressure functions. Different residual saturations or minimum wetting fluid saturations can not be assigned in the TETRAD code. The Operable Unit 7-13/14 benchmark problem (EX3DT) moisture characteristics provided to GeoTrans were used in this problem.

Default carbon tetrachloride chemical functions were used in the T2VOC simulation and the exact values used for the simulated pressure and temperature were not provided by the GeoTrans personnel. The T2VOC parameters provided were for functional relationships of Henry's constant, diffusivity, viscosity, and vapor pressure. The functional relationships were provided in the form of FORTRAN source code. A large amount of time would be needed to determine the exact values used by T2VOC, because both the subroutine and callings source code must be examined to determine how the calculated variables returned to the main program are used. Instead, the TETRAD phase equilibrium parameters were selected for isothermal conditions (20 degrees C) and standard pressure (1 atm) from published values.

The simulation results illustrate the carbon tetrachloride spreading laterally above the low permeability clay layer and moving down vertically through the gap. Eventually, the carbon tetrachloride reaches the water table and begins to move left to right with in the direction of aquifer flow. No numerical problems were encountered and the simulation carbon tetrachloride relative mass balance error was 1.e-6. Notable differences between the TETRAD and T2VOC simulation results are the TETRAD simulation predicts more lateral carbon tetrachloride movement above the clay layer than the T2VOC simulations. The vertical migration of the carbon tetrachloride is very similar in between the two simulation results. Figures 21 through 23 illustrate the left to right vertical water phase concentration through the carbon tetrachloride release location at 365, 730, and 255 days; respectively. Table 21 provides the water phase concentration with time at 5 locations in the model. Figure 24 illustrates the concentration with time at the same locations.

Table 20. TETRAD simulation parameters for the carbon tetrachloride benchmark problem.

Parameter	Sand Value	Clay Value
Porosity	0.48	0.15
Horizontal Permeability (mD)	3500	1
Vertical Permeability (mD)	700	1
Residual Water Saturation	0.15	0.25
Residual Gas Saturation	0.0	0.0
Residual Oil Saturation	0.008	0.008
TETRAD ALP Parameter	2.0	1.5
TETRAD BET Parameter	1.8	1.2
TETRAD GAM Parameter	0.0	0.0
TETRAD SIGOW Parameter	1.0	1.0
TETRAD SIGGO Parameter	0.0	0.0
TETRAD SIGGW Parameter	1.0	1.0
Water Liquid Density (Kg/m^3)	1000.	
DNAPL Liquid Density (Kg/m^3)	1584.	
Water Viscosity (mPa S)	1.0	
DNAPL Viscosity (mPa S)	1.0	
Temperature (degree C)	20.	

Parameter	Sand Value	Clay Value
Water Phase Diffusion Coefficient (m^2/day)	7.2e-5	
Water Phase Tortuosity	2.0	
Gas Phase Diffusion Coefficient (m^2/day)	0.72	
Gas Phase Tortuosity	Millington (1959) Relationship	
Organic Partition Coefficient (mL/g)	439	
Fraction of Organic Carbon	0.001	
NAPL Vapor Pressure (mmHg)	87	
NAPL Henry's Law Constant (non-dimensional)	0.965	

Table 21. Carbon tetrachloride water phase concentration with time at 5 observation points.

Time (days)	Concentration (Kg/m^3) at x=8, y=1, z=3	Concentration (Kg/m^3) at x=8, y=1, z=8	Concentration (Kg/m^3) at x=8, y=1, z=13	Concentration (Kg/m^3) at x=12, y=1, z=18	Concentration (Kg/m^3) at x=18, y=1, z=21
0.000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
1.000	7.572e-001	1.795e-009	8.888e-026	0.000e+000	0.000e+000
10.000	7.572e-001	1.239e-004	1.008e-015	1.171e-021	0.000e+000
45.000	7.572e-001	1.837e-002	3.444e-010	6.743e-013	5.965e-026
91.000	7.572e-001	8.802e-002	5.384e-008	7.213e-010	8.537e-021
182.000	7.572e-001	2.145e-001	4.393e-006	3.247e-007	2.718e-015
273.000	7.572e-001	3.188e-001	3.068e-005	4.367e-006	5.333e-013
365.000	7.572e-001	4.111e-001	9.486e-005	1.880e-005	8.631e-012
456.000	7.572e-001	4.444e-001	2.051e-004	4.991e-005	5.657e-011
547.000	7.572e-001	5.076e-001	3.735e-004	1.085e-004	3.299e-010
639.000	7.572e-001	5.854e-001	5.965e-004	2.008e-004	1.504e-009
730.000	7.572e-001	6.033e-001	8.631e-004	3.265e-004	5.435e-009
821.000	7.572e-001	7.085e-001	1.162e-003	4.794e-004	1.419e-008
912.000	7.572e-001	7.187e-001	1.478e-003	6.623e-004	3.418e-008
1004.000	7.572e-001	7.204e-001	1.812e-003	8.717e-004	7.452e-008
1095.000	7.572e-001	7.221e-001	2.137e-003	1.085e-003	1.470e-007
1186.000	7.572e-001	7.281e-001	2.444e-003	1.308e-003	2.641e-007
1277.000	7.572e-001	7.478e-001	2.726e-003	1.530e-003	4.410e-007
1369.000	7.572e-001	7.572e-001	3.000e-003	1.752e-003	6.939e-007
1460.000	7.572e-001	7.572e-001	3.247e-003	1.966e-003	1.026e-006
1551.000	3.649e-001	7.572e-001	3.487e-003	2.179e-003	1.453e-006
1642.000	3.615e-001	7.572e-001	3.709e-003	2.384e-003	1.983e-006
1734.000	3.649e-001	7.572e-001	3.914e-003	2.581e-003	2.615e-006
1825.000	3.675e-001	7.572e-001	4.102e-003	2.769e-003	3.359e-006
1916.000	3.709e-001	7.572e-001	4.282e-003	2.948e-003	4.196e-006
2007.000	3.735e-001	7.572e-001	4.452e-003	3.119e-003	5.119e-006
2099.000	3.760e-001	7.572e-001	4.615e-003	3.290e-003	6.145e-006

Time (days)	Concentration (Kg/m^3) at x=8, y=1, z=3	Concentration (Kg/m^3) at x=8, y=1, z=8	Concentration (Kg/m^3) at x=8, y=1, z=13	Concentration (Kg/m^3) at x=12, y=1, z=18	Concentration (Kg/m^3) at x=18, y=1, z=21
2190.000	3.786e-001	7.572e-001	4.769e-003	3.444e-003	7.230e-006
2281.000	3.803e-001	7.572e-001	4.922e-003	3.598e-003	8.367e-006
2372.000	3.829e-001	7.572e-001	5.068e-003	3.743e-003	9.572e-006
2464.000	3.854e-001	7.572e-001	5.213e-003	3.888e-003	1.085e-005
2555.000	3.871e-001	7.572e-001	5.350e-003	4.025e-003	1.205e-005

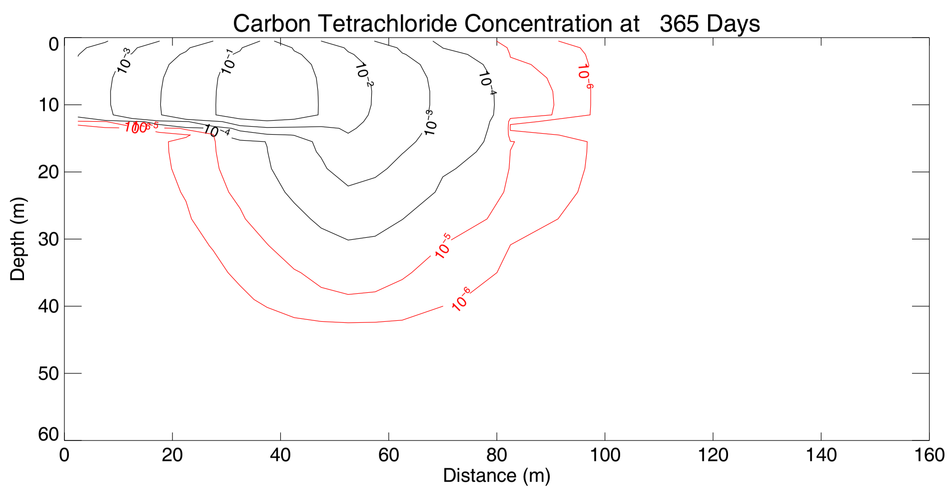

Figure 21. Vertical carbon tetrachloride water phase concentration (Kg/m^3) through source area after 365 days.

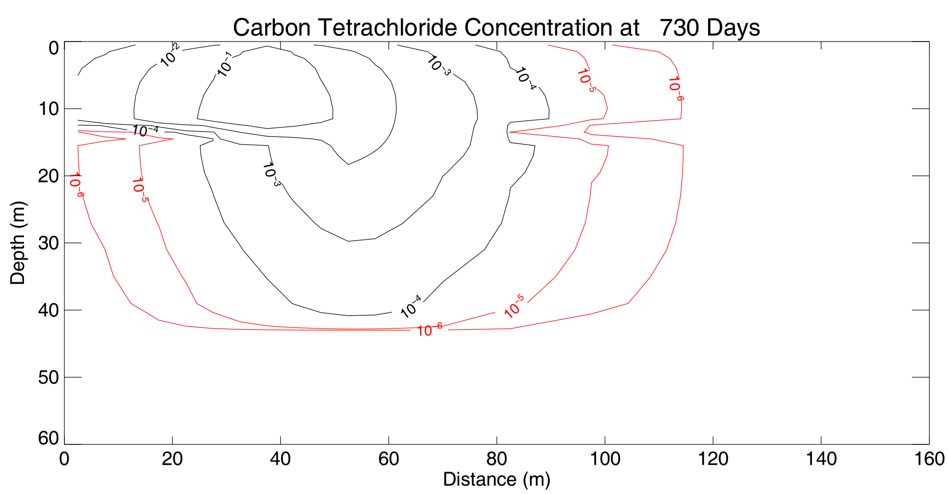

Figure 22. Vertical carbon tetrachloride water phase concentration (Kg/m^3) through source area after 730 days.

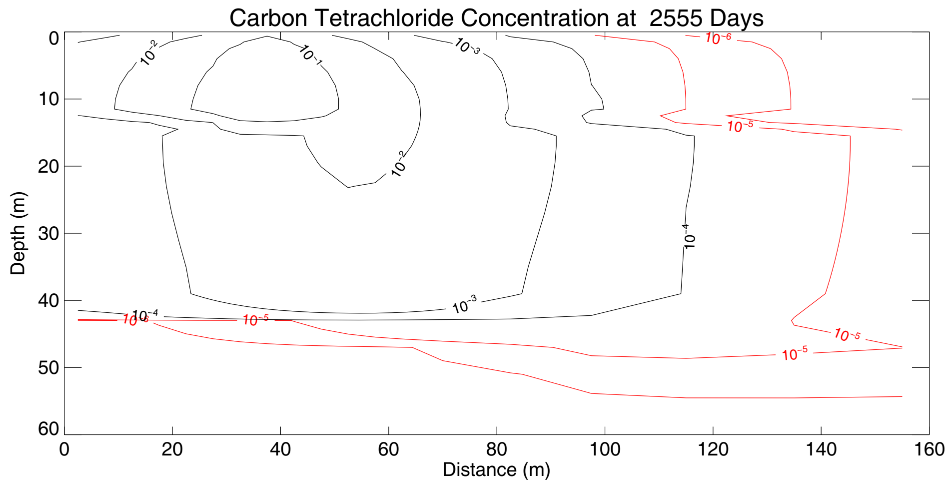

Figure 23. Vertical carbon tetrachloride water phase concentration (Kg/m^3) through source area after 2555 days.

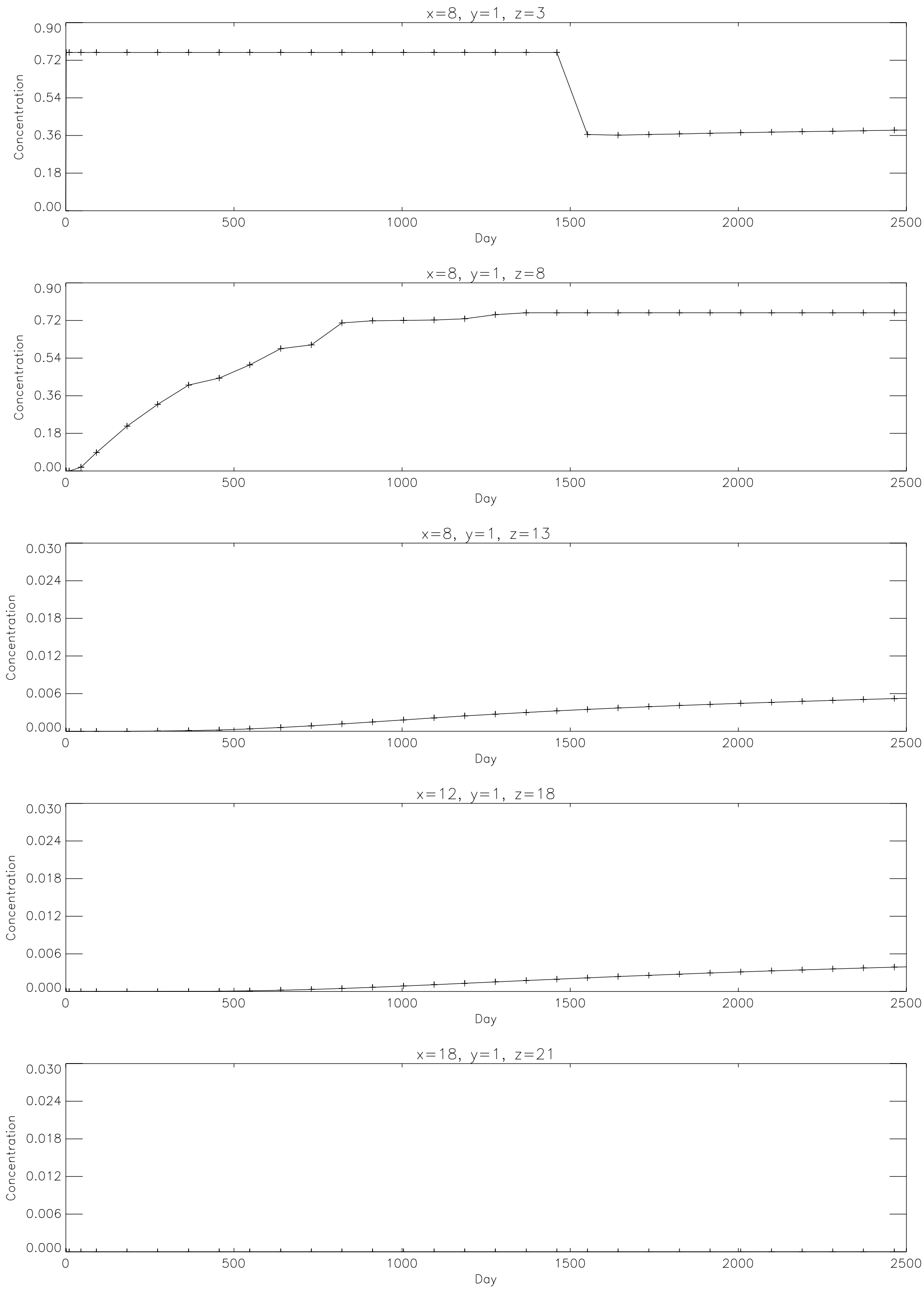

Figure 24. Carbon tetrachloride water phase concentration (Kg/m^3) with time at 5 observation points.

11 CONCLUSIONS

Most of the problems simulated in this verification and benchmarking study, except problems EPA 2D and EPA 2F, are best suited for a conventional simulator that solves the fluid mass and energy conservation equations separately from the transport conservation equations. The conventional simulators solve the flow field first and then use the velocities for a separate transport solution. This can not be done with the TETRAD simulator because the solute is tracked as a fluid component, which participates in the flow solution.

This benchmarking exercise illustrates that the TETRAD code can be used as an environmental simulator, if very dilute dissolved contaminants concentrations are scaled up (often many orders of magnitude) to a reasonable mass fraction for maintaining mass balance, while still maintaining small enough concentrations as to not affect the water pressure during sorption or radioactive decay. This requires additional care in preparing simulation input, monitoring simulation mass balance, verifying accurate results, and post-processing simulation output. The radionuclide chain decay problems were particularly difficult to implement in the TETRAD simulator because of the following factors:

- These simulations required using the ‘BVMULT’ keyword to multiply the source area grid block volume by a large factor (1e+10). This requires very good overall mass balance to resolve the nuclide within the model domain down gradient of the source.
- The mass concentration difference between the parent and daughter nuclides could range over five orders of magnitude. This requires an accurate solution over a large range of concentrations. The TETRAD simulator requires the radionuclides by simulated in mass concentration instead of activity concentration. This is required to conserve total mass in the parent to daughter decay process.
- The radionuclides were sorbing. This required scaling concentrations to a small mole fraction in the simulation domain down gradient of the sources.

The combination of the factors discussed above often required the relative mass balance error to be less than 1.e-10 magnitude to maintain an accurate solution.

The simulations presented in this report were performed without prior knowledge of the benchmark solutions. Agreement with the benchmark code could be improved with model grid, boundary condition, time step control, and convergence tolerance refinement.

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